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Semiannual Report

October 1, 2001 through March 31, 2002

August 2002

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INTRODUCTION

ICASE* is operated at the Langley Research Center (LaRC) of NASA by the Universities Space Research Association (USRA) under a contract with the Center. USRA is a nonprofit consortium of major U.S. colleges and universities.

The Institute conducts unclassified basic research in applied mathematics, numerical analysis and algorithm development, computer science, fluid mechanics, and structures and materials in order to extend and improve problem-solving capabilities in science and engineering, particularly in the areas of aeronautics and space research.

ICASE has a small permanent staff. Research is conducted primarily by its permanent staff and visiting scientists from universities and industry who have resident appointments for limited periods of time as well as by visiting and resident consultants. Members of NASA's research staff may also be residents at ICASE for limited periods.

The major categories of the current ICASE research program are:

- Applied and numerical mathematics, including multidisciplinary design optimization;
- Applied computer science: system software, systems engineering, and parallel algorithms;
- Theoretical, computational, and experimental research in fluid mechanics in selected areas of interest to LaRC, such as transition, turbulence, flow control, and acoustics; and
- Theoretical, computational, and experimental research in structures and material sciences with emphasis on smart materials and nanotechnologies.

ICASE reports are primarily considered to be preprints of manuscripts that have been submitted to appropriate research journals or that are to appear in conference proceedings. A list of these reports for the period October 1, 2001 through March 31, 2002 is given in the Reports and Abstracts section, which follows a brief description of the research in progress.

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RESEARCH IN PROGRESS

APPLIED AND NUMERICAL MATHEMATICS

Numerical Simulation of Embedded Streamwise Vortices in a Turbulent Boundary Layer

Brian Allan

The use of low-profile vortex generating vanes, which are only a fraction of the boundary layer thickness, has been shown to be more efficient than standard-sized vanes, for some passive flow control applications. Like the standard size vortex-generating vanes, which are typically the same height of the boundary layer thickness, the low-profile vanes still provide effective momentum transfer while having a reduced residual drag. These low-profile vanes are currently being investigated for improving engine face flow distortion for compact S-shaped inlets. Unlike the standard-size vanes, the low-profile vanes produce streamwise vortices which are embedded in the boundary layer. The design of inlets and other aerospace applications, which use low-profile vortex generators, need to rely on the ability to model and simulate these devices. This investigation will evaluate the ability of a Reynolds averaged Navier-Stokes (RANS) code to simulate an embedded streamwise vortex, generated by a low-profile vane, fixed on a flat plate by comparing numerical simulations to experimental data.

Using a compressible RANS code, developed at NASA, numerical simulations of a single low-profile vortex generator vane on a flat plate, have been performed. These simulations were conducted in coordination with experiments at NASA Langley's 20x28-inch Shear Flow Tunnel. Comparisons of the numerical results to the experimental data for the single vane, have shown that the turbulence modeling has a significant effect on the computed flow field. A comparison between numerical simulations using a Spalart-Allmaras (SA) and a Mentor SST model was made to the experimental results. This comparison showed the embedded streamwise vortex in the simulations to be more dissipated than was observed in the experiments. However, the simulation using the SST model was able to predict the trajectory of the vortex core and the peak vorticity, better than the SA model. A comparison of circulation showed that the numerical simulations using the SST and SA turbulence models, generated vortices of equal strength. Therefore, the lower peak vorticity using the SA model is related to the larger turbulent eddy viscosity predicted by the SA model. In general the SST turbulence model was able to predict the trajectory and circulation strength of the streamwise vortex. However, both numerical simulations were shown to diffuse the vortex much faster than observed in experiments.

Future work will include detailed experiments using both low-profile and standard-size vanes at different device angles on a flat plate. These wind tunnel experiments will be compared to numerical simulations providing better insight into the physics and modeling of vortex generating vanes.

This work was done in collaboration with Pieter Buning, Chung-Sheng Yao, and John Lin (NASA Langley). Numerical results were computed using the ICASE PC cluster, Coral.

Feedback Flow Control Design for Inlet Flows

Brian Allan

In order to increase the performance of inlet flows for varying flow conditions, active flow control devices for a S-duct inlet design are being investigated at the NASA Langley Research Center, under the UEET program. One of the active flow control devices being considered are vortex generating jets. Unlike fixed vanes, these devices can be turned on and off when needed. By incorporating the jets with a feedback

controller, it is desired that the performance of a S-shaped inlet will be improved over a wider range of flow conditions. By using computational fluid dynamics (CFD) the performance of the jets, as well as the placement of sensors and actuators, can be explored. CFD will also be used to model, design, and evaluate the closed-loop flow control system for the S-duct inlet.

The inlet flow is simulated using a compressible Reynolds averaged Navier-Stokes code developed at NASA. Numerical simulations for the baseline flow of a rectangular duct with an expanding cross section have already been performed and compared to experiments conducted at NASA Langley. The numerical simulations were able to capture the characteristics of the flow separation pattern but were unable to get the exact location of the vortex lift off locations and stagnation points. However, the CFD simulations were able to match the surface pressure on the upper and lower surface of the duct for the baseline case. Time accurate simulations of vortex generating jets on a periodic ramp have also been performed. These time accurate simulations have been used to develop a model of this flow system which was then used in the feedback controller design. The objective of this control design was to improve the surface pressure gradient on the ramp. Once the feedback controller was designed, it was then simulated by coupling the CFD with the control system. The results and experiences from the periodic ramp problem are being used to model and design a flow control system for the S-duct inlet which will provide guidance for a flow control experiment at NASA Langley.

Future work will involve baseline simulations of the inlet which will then be followed by adding flow control actuators. Once these simulations are performed the flow system can be modeled and a feedback controller designed. These simulations are being performed in conjunction with wind tunnel experiments at NASA Langley and will be compared to the wind tunnel results.

This work was done in collaboration with Pieter Buning and Susan Gorton (NASA Langley). Numerical results are computed using the ICASE PC cluster, Coral.

Real Time Computational Algorithms for Eddy-current-based Damage Detection

H.T. Banks

In the field of nondestructive evaluation, new and improved techniques are constantly being sought to facilitate the detection of hidden corrosion and flaws in structures such as aeroplanes and pipelines. In recent efforts, we explored the feasibility of detecting such damage by application of an eddy-current-based technique coupled with reduced order modeling.

We first developed a model for a specific eddy current method in which we make some simplifying assumptions reducing the three-dimensional problem to a two-dimensional problem (we do this for proof of concept). Theoretical results are then obtained that establish the existence and uniqueness of solutions as well as continuous dependence of the solutions on the parameters which represent the damage. A least squares parameter estimation problem was used in identifying the geometry of the damage.

To solve the identification problem, an optimization algorithm was employed which requires solving the forward problem numerous times. To implement these methods in a practical setting, the forward algorithm must be solved with extremely fast and accurate solution methods. In constructing these computational methods, we employed reduced order proper orthogonal decomposition (POD) techniques. This approach permits one to create a set of basis elements spanning a data set consisting of either numerical simulations or experimental data. We developed two different algorithms for forming the POD approximations, a POD/Galerkin technique, and a POD/interpolation technique.

Finally, results of the inverse problem associated with damage detection were obtained using both sim-

ulated data with relative noise added as well as experimental data obtained using a giant magnetoresistive sensor. The experimental results are based on successfully using experimental data to form the POD basis elements (instead of numerical simulations), thus illustrating the effectiveness of this method on a wide range of applications. In both instances the methods are found to be efficient and robust. Moreover, the methods were fast; our findings demonstrate a *significant* reduction (by factors of order 10^3) in computational time.

This research represents continuing joint effort with Michele L. Joyner (North Carolina State University) and Buzz Wincheski and William P. Winfree (NDES, NASA Langley).

Feedback Control of Nonlinear Systems

Scott C. Beeler

We are studying the feedback control of nonlinear systems of ODEs, in particular using the state-dependent Riccati equation (SDRE) method. We are especially interested in this technique because it is based on optimal control conditions and so its control performance should be very good compared to other methods. It is based on the simple form of linear Riccati control solutions while seeking to incorporate as much of the nonlinear nature of the problem as possible. This may prove useful in aircraft guidance and control problems including control actuator impairment situations. We also are studying the flight dynamics of small remote-controlled gliders in an ambient wind field. With unpowered flight the aircraft has a smaller velocity, and so the winds have a greater effect on the aircraft's flight properties. This can work in its favor, since with efficient control laws the aircraft can extract energy from thermals or wind gradients to stay aloft for long periods of time without needing fuel to run an engine. The research objective is to develop new nonlinear control techniques with good performance and robustness properties, and to study the flight properties of small gliders to evaluate their potential for long-term flight.

We have continued to test our Matlab SDRE feedback control algorithms on example problems with state and control nonlinearities, obtaining good results while modifying the several versions of the SDRE method we have implemented. An application to a highly nonlinear inverted pendulum control problem is presently being performed, and it has necessitated some alterations in the algorithm to counter the more complex nature of this example problem. The glider model has been fine-tuned, and its Matlab and Fortran implementations tested. Some very good preliminary results have been achieved for the scenario of minimizing altitude loss while traveling from point to point through a wind field. The results achieved for both the SDRE and glider codes show the efficiency of the techniques used, and are encouraging as we move on to further complex application problems and look to combine these newly developed algorithms with established techniques to improve their desirable properties.

Future efforts include application of the SDRE method to other realistic examples such as aircraft guidance problems, possibly a version of the small glider model. It may also be combined with other control methods to improve its robustness while retaining its desirable control efficiency. The refined glider model will be further tested, using optimal control techniques and later feedback control. Once these small-scale control trials have been completed, larger-scale glider surveying problems can be studied, possibly combining the small-scale feedback controls with fuzzy logic control for decision-making processes.

This work is done in collaboration with D. Moerder and D. Cox (NASA Langley, Guidance and Control Branch).

Study of the Flux Retrieval Error Behavior with CERES/TRMM Data

A. Bodas-Salcedo

The Earth Radiation Budget is a fundamental quantity in climate studies, which on a global scale can only be measured with sufficient accuracy from satellites. Radiometers onboard satellites carry out directional measurements (radiances), but the physical quantity of interest to obtain the radiation budget is the flux density, which is the hemispherical integral of the radiance field. Therefore, the development of inversion algorithms (anisotropic models) to retrieve the flux estimate from radiance measurements is needed. The purpose of this work is to study the dependency of the error of flux retrieval algorithms with respect to the observing geometry.

In order to carry out this study, following tasks have been developed:

1. Analysis of 14 days of CERES/TRMM data (CERES stands for Clouds and the Earth's Radiant Energy System, and TRMM for Tropical Rainfall Measuring Mission), by sorting radiance measurements in angular and cloud cover bins, both in shortwave and longwave bands, and building a database at different time scales.
2. With the previous database, sampling problems that will impact the construction of anisotropic models have been investigated.
3. Shortwave (SW) and longwave (LW) anisotropic models have been built, and a methodology to study the performance of the anisotropic models has been developed.
4. That methodology has been applied to study the flux retrieval error dependency with the observing geometry.

Following this approach, we have demonstrated that a privileged region in the flux retrieval algorithm appears in the region of viewing zenith angles around 55 degrees, giving the possibility to obtain top of the atmosphere flux estimates with good accuracy and simple anisotropic models by selecting properly the observing geometry.

Although only a few days of CERES/TRMM data have been processed, it seems promising to continue this line of investigations by using the whole CERES/TRMM record, in order to minimize sampling problems which still may be affecting our results. Furthermore, cloud optical depth should be introduced in the scene definition so that a more accurate error analysis may be carried out.

This research was conducted in collaboration with G.L. Smith (Virginia Polytechnic Institute and State University) and E. López-Baeza (Universidad de Valencia, Spain).

Textbook Multigrid Efficiency for CFD Simulations

Boris Diskin

An efficiency goal for the new generation of multigrid flow solvers is to arrive at solutions of the governing system of equations in a total computational work that is a small (less than 10) multiple of the operation count in one target-grid residual evaluation. Such efficiency is defined as textbook multigrid efficiency (TME). TME for the Navier-Stokes simulations can be achieved if different factors contributing to the system could be separated and treated optimally, e.g., by multigrid for elliptic factors and by downstream marching for hyperbolic factors. An efficient way to separate the factors is the distributed relaxation approach. Design of a distributed relaxation scheme can be significantly simplified if the target discretization is factorizable, i.e., possessing the following two properties:

(1) The determinant of the (principally) linearized discrete operator can be represented as a product of discrete scalar factors, each of them approximating a corresponding factor of the determinant of the

differential Navier-Stokes equations.

(2) The obtained scalar factor discretizations are stable, easily solvable, and reflect the physical anisotropies. Recently, a family of factorizable discretization schemes for the compressible flow equations has been developed. The goal of my research performed in the last six months was to analyze these new schemes. In particular, I have been focused on discretization of boundary conditions and correct combination of the different parts of a multigrid solver to provide a TME solution for the Navier-Stokes equations in different flow regimes.

A detailed discrete analysis has been employed to evaluate several sets of boundary conditions for factorizable schemes corresponding to the steady-state compressible Euler equations. Requirements for practical boundary conditions have been formulated. Several sets of practical boundary conditions have been tested and compared with overspecified boundary conditions. The effects of boundary-condition equations on stability and accuracy of the discrete solutions have been analyzed. Explicit correspondence between solutions and boundary conditions has been established through a boundary-condition-sensitivity (BCS) matrix. Analysis of coefficients of the BCS matrix provides reliable predictions for stability and accuracy of the discrete solutions. The following new findings are reported:

(1) Examples of stable discrete problems contradicting a wide-spread belief that employment of a one-order-lower approximation scheme in an $O(h)$-small region does not affect the overall accuracy order of the solution have been found and explained. Such counterexamples can only be constructed for systems of differential equations. For scalar equations, the conventional wisdom is correct.

(2) A negative effect of overspecified (although, exact) boundary conditions on accuracy and stability of the solution has been observed and explained.

(3) Sets of practical boundary conditions for the new factorizable schemes have been formulated. These schemes belong to a family of second-order schemes requiring second-order accuracy for some numerical-closure boundary conditions.

The BCS-matrix analysis has also been applied for formulating suitable interface boundary conditions for the local relaxation procedure complementing distributed relaxation sweeps in a TME solver for the compressible Euler equations. Accurate and stable supplemental boundary conditions for pressure required for solution of the incompressible Navier-Stokes equations in the pressure-equation formulation have also been derived by means of this analysis. This analysis has been very instrumental for recent TME demonstrations in solving collocated-grid discretizations of the Euler and Navier-Stokes equations.

Currently the efforts are directed to demonstrate TME for general flow computations including general boundary conditions and captured shocks.

This research was conducted in collaboration with J.L. Thomas (NASA Langley).

Atmosphere Modeling Efforts for 2001 Mars Odyssey Aerobraking

Alicia Dwyer

In October 2001, the Odyssey Spacecraft began aerobraking operations at Mars. Aerobraking uses the atmosphere of a planet rather than chemical propulsion to reduce the size of the orbit. The success of aerobraking depends on the characterization of parameters that affect the safety of the spacecraft. These parameters include primarily aerodynamic forces and atmospheric density. Variations in atmospheric density constitute the largest orbit-to-orbit uncertainty. Therefore it was desirable to develop models of the atmospheric density that accurately predict density at aerobraking altitudes. Predictions of the atmosphere influence maneuver decisions and therefore affect the duration of the aerobraking mission and the amount

of fuel required.

Throughout the 77 days of aerobraking daily models of the atmosphere were developed. The models were based on comparisons between the onboard accelerometer derived density and the Mars Global Reference Atmosphere Model (Mars-GRAM) calculated density. Mars-GRAM was also used as the basis for the navigation predictions. The density versus time profiles for both the accelerometer and model densities were produced for each orbit. Ratios of accelerometer to Mars-GRAM data were obtained for maximum and periapsis densities and changes in velocity. Wave models were produced using a least squares fit to a selected number of ratios. Because of the large variability in the Mars atmosphere it was not possible to rely on a single wave model for extended periods of time (i.e., weeks). For this reason the aerobraking wave modeling effort included the analysis of stationary and moving wave models, the effects of using different wave numbers, and the optimization of the number of orbits in each fit. The model that produced the best fit for a given set of orbits was then used to provide predictions for subsequent orbits. Despite the large variability in the Mars atmosphere and the fact that no single model was able to capture the local and daily changes for extended periods of time, the modeling efforts proved instrumental in the maneuver decisions made throughout aerobraking.

All the data collected during aerobraking using the accelerometers and the atmospheric modeling efforts is being archived and will be used to update current models for future missions to Mars.

The atmospheric modeling work was done in collaboration with Dr. Robert Tolson and Mr. Gerald Keating (George Washington University).

Development of Aeroassist Capabilities for Planetary Orbit

Jill Hanna

Propulsive maneuvers to enter into planetary orbit have been designed since the beginning of space exploration. However, to reduce fuel usage and launch mass, more economical approaches for capture into planetary orbit have been studied recently. The use of a planetary atmosphere to reduce the orbital energy of a spacecraft is the most cost efficient capture strategy to date. One aeroassist strategy, atmospheric aerobraking, has been used successfully in three different planetary missions, Magellan at Venus, Mars Global Surveyor, and the most recent Mars 2001 Odyssey to change an elliptical orbit to a nearly circular orbit. Other methods of aeroassist such as aerocapture are also being studied to reduce the time required to modify the spacecraft's orbital trajectory.

Mars 2001 Odyssey was the most recent aerobraking success. During the 77-day aerobraking phase between October 2001 and January 2002, accelerometer derived density profiles were developed and used for atmospheric estimations. The atmosphere was modeled to improve predictive techniques. Three degree of freedom (dof) and six dof flight simulations were performed to reproduce and predict the trajectory of Odyssey throughout the atmosphere of Mars. Through the six dof work, it was determined that there was a significant amount of impingement of the reaction control system thrusters on and around the spacecraft, yielding more fuel usage required for the desired effect from the thrusters. The success of Odyssey has had a significant impact on future planetary exploration. Odyssey has returned valuable atmospheric data that will be useful for future Mars aeroassist opportunities. The science data that is collected from Odyssey will aide in choosing landing sites for future missions. The next Mars orbiter is the 2005 Mars Reconnaissance Orbiter (MRO). Research is being performed to incorporate the successful Mars Odyssey techniques. The research done with MRO will be useful in determining the length of MRO aerobraking and will improve and make more autonomous the aerobraking work supplied by NASA Langley to the Jet Propulsion Laboratory.

Other exploration using aeroassist includes a Titan aerocapture mission. The feasibility of a ballute system is being studied and traded with aerocapture using only a heat shield for drag effect. This research will help to determine the size, shape, and mass properties of a ballute system.

Future work includes further improving MRO aerobraking software, changing all software to an updated version of programming code, and producing mission runouts and aerobraking statistics. MRO aerobraking is scheduled to begin in March 2006 and last for five months.

Unstructured Nonconforming Multigrid Algorithms for the Solution of Radiation Transport Problems

Kab Seok Kang

The simulation of radiation transport in the optically thick flux-limited diffusion regime has been identified as one of the most time-consuming tasks within large simulation codes. Due to multimaterial complex geometry, the radiation transport system must often be solved on unstructured grids. A variety of finite volume and conforming finite element schemes have been employed in research at ICASE and at numerous national laboratories on this so-called "radiation diffusion" system. Meanwhile, multilevel nonconforming finite element or covolume methods have proven flexible and effective on incompressible fluid flow problems. The objective of this research is to investigate the behavior and the benefits of unstructured nonconforming multigrid algorithms used as linear solvers (inside of Newton approaches), directly as nonlinear solvers, or simply as preconditioners in solving steady and unsteady implicit radiation diffusion problems.

We have completed debugging code of linear versions of a two-dimensional unstructured nonconforming multigrid algorithm and have begun to write a report about the behavior and the benefits of the unstructured P_1 nonconforming finite element method and comparisons with some linearization methods and parallelization. We use the P_1 nonconforming finite element space on triangular mesh and nested-mesh subdivision to automatically generate a sequence of unstructured meshes on the domain and found the P_1 nonconforming finite element method of radiation transport problem on inhomogeneous domains resolve very sharp changes of energies near the layer where the two different materials meet.

We plan to measure its scalability on large numbers of processors on the ICASE Beowulf system and other machines, and extend into three-dimensional settings.

Robust Optimization Under Uncertain Design Conditions

Wu Li

The ultimate goal is to develop next-generation design tools that are insensitive to variability or uncertainty in design specifications. One important example is aerodynamic shape optimization for achieving drag reduction under uncertain flight conditions. Our objective is to use both deterministic and probablistic strategies in optimization process to avoid undesirable decisions made by an optimizer due to a lack of information under the uncertain flight conditions.

A combination of the expected value optimization and the profile optimization is developed to give users trade-off options between a greedy reduction of the average drag or a consistent reduction of the drag over the range of the uncertainty parameter. This new method is called the constrained multipoint approximation method (CMAM) for robust airfoil optimization. CMAM is tested on a lift-constrained drag minimization problem for a two-dimensional airfoil in Euler flow, which is formulated with 20 free design variables. Each free design variable is the y-coordinate of a control point in the B-spline representation of the airfoil shape. An unstructured grid computational fluid dynamics code, FUN2D, is used to compute

the lift/drag coefficients and their gradients with respect to airfoil shapes and angles-of-attack. Hermite spline interpolation formula is used to estimate the expected value of the drag over the Mach range. A parallel implementation of CMAM using MPI library reduces the walltime of each optimization iteration to one function and one gradient evaluation no matter how many design points are used. Special modifications of the standard trust region optimization strategy are used to reduce potential random shape distortions during the optimization process. Also, due to difficulty or impossibility of obtaining accurate derivatives for aerodynamic quantities, we are also working on a derivative-free optimization (DFO) method for robust airfoil shape optimization.

In the last two years, researchers at ICASE have developed the expected value optimization method and the profile optimization method for robust airfoil optimization under uncertain flight conditions. The expected value optimization method uses a dynamic numerical approximation of the expected value of the drag to avoid off-design degradation problems encountered by the traditional multipoint optimization method, while the profile optimization method uses a smart descent direction to achieve a consistent drag reduction over the entire Mach range and search for a robust optimal solution. By selecting various ratios of two input control parameters, CMAM can generate optimal solutions corresponding to the multipoint optimization method, the expected value optimization method, the profile optimization method, and a combination of all these methods, respectively. This shows how these different optimization methods are related to each other. The numerical simulation results indicate that CMAM is flexible for testing and comparing various robust optimization strategies. By using a special trust region strategy, it generates intermediate iterates without any undesirable noises in airfoil shapes, no matter what optimization strategy is used. With only four design points, CMAM generates smooth optimal airfoils with smooth drag profiles over the given Mach range. Optimization techniques can automate many design tasks, providing better designs in a shorter time. However, traditional optimization methods require precise specification of the objectives and constraints. By contrast, robust optimization methods allow uncertainty in design specifications. However, when there is a nonlinear uncertainty parameter in the optimization model, one could only solve an approximation model of the original optimization problem. Each approximation method has its own strength and weakness. Some methods allow a designer to explore the design space, while others generate improved designs using the smallest possible change in the baseline configuration. It is critical to be able to analyze and compare various techniques for robust optimization involving highly nonlinear objective/constraint functions with respect to the uncertainty parameter (such as the drag with respect to the Mach number). CMAM uses a general optimization model to encompass all existing robust optimization methods for airfoil shape optimization under uncertain flight conditions and allows a systematic study of various robust airfoil optimization methodologies.

CMAM will be extended to study airfoil shape optimization with multiple uncertainty parameters. In collaboration with ICASE, the mathematical properties of the method will be analyzed in order to generalize the method for use in future MDO applications. In collaboration with Michael Wagner, we will also develop DFO methods to deal with more realistic and complex aerodynamic shape optimization problems.

This research was conducted in collaboration with Sharon Padula (NASA Langley) and Michael Wagner (Old Dominion University and ICASE).

The Coral Project

Josip Lončarić and Manuel D. Salas

The cost of developing complex computer components such as CPUs has become so high that scientific applications alone cannot carry the full burden. Scientific computing needs to use mass market leverage

to overcome the cost barrier. A cost-effective alternative to high-end supercomputing was pioneered by Beowulf, a cluster of commodity PCs. By now, very high performance Beowulf clusters can be built using fast commodity PCs and switched Fast Ethernet. We are exploring the benefits and the limitations of this approach, based on applications of interest to ICASE.

The initial phase of the Coral project, consisting of 32 Pentium II 400 MHz nodes and a dual-CPU server, demonstrated aggregate peak performance in excess of 10 Gflop/s, with sustained performance on CFD applications of about 1.5 Gflop/s. In order to provide a richer environment for further experimentation, a dual-CPU configuration was chosen for the second phase of the Coral project. We have added 16 dual Pentium III 500 MHz machines and two dual-CPU file servers. The third stage of this project added 16 dual Pentium III 800 MHz machines and a 32-node low latency 1.25 Gbps Giganet cLAN network fabric. This year the project is in its fourth stage, and 24 of the original 400 MHz machines were replaced with much faster 1.7 GHz machines. The resulting system contains 96 compute CPUs and 7 server CPUs with an aggregate of nearly 55 GB of RAM and 2 TB of raw disk space. Coral has an excellent price/performance ratio, almost an order of magnitude better than an equivalent proprietary supercomputer design. This conclusion is based on our experience with a variety of applications, ranging from coarse-grained domain decomposition codes to communication-intensive parallel renderers. Coral has computed solutions to many large scale problems, and users needed a filesystem large enough to store their output. Therefore, we have converted one of the original 400 MHz machines into a file server with a RAID-5 array consisting of four 160 GB ATA/133 disks. The formatted capacity of this new filesystem is 481 GB (where GB=10^9 bytes). This RAID-5 array can read data at 66 MB/s. The file server has been observed to deliver up to 35 MB/s when serving multiple nodes via the Gigabit Ethernet interface using the NFS protocol. The incremental cost of this file server was only \$2.24/GB of filesystem space.

We will continue to use this cluster to develop and run research codes of interest to ICASE and NASA Langley, and to evaluate price/performance tradeoffs among various hardware, software, and networking configurations.

Active Shielding and Optimal Control of Environmental Noise

Josip Lončarić and Semyon V. Tsynkov

Rejection of exterior noise caused by periodic sources such as propellers or turbines would significantly enhance passenger comfort and reduce noise fatigue on long flights. Passive sound absorbing materials help at high frequencies, but to be effective below about 1 kHz their weight penalty becomes significant. Active noise control can reduce low frequency noise with less weight penalty. Based on the mathematical foundations of a new active technique for control of the time-harmonic acoustic disturbances, we have developed a numerical technique which can suggest good locations for sensors and actuators.

Unlike many existing methodologies, the new approach provides for the exact volumetric cancellation of the unwanted noise in a given predetermined region of space while leaving those components of the total sound field deemed as friendly unaltered in the same region. Besides, the analysis allows us to conclude that to eliminate the unwanted component of the acoustic field in a given area, one needs to know relatively little: only the perimeter data (the total acoustic field and its normal derivative) are required. The mathematical apparatus used for deriving the general solution is closely connected to the concepts of generalized potentials and boundary projections of Calderon's type. This exact general solution can be computed at polynomial cost, and good actuator locations determined via a procedure which progressively restricts the locations where actuators may be placed. The answer depends on the chosen optimality criterion. While L_2 optimality of

control inputs is typically sought, this criterion is not physically meaningful. Minimizing the L_1 norm of the control effort has a clear physical interpretation, but it is very difficult to solve numerically. Fortunately, our numerical results for the two-dimensional case and our analytic proof for the 1-D case show that perimeter controls are L_1 optimal. This is a strong basis for our conjecture that perimeter controls are L_1 optimal in general. Finally, we've shown that noise control can absorb power. The power optimal controls load the noise sources to increase their power output, then absorb half of the power increase as the other half radiates to infinity.

These results on L_2 optimality, L_1 optimality and power optimality provide useful guidance for the exact volumetric cancellation of noise. We plan to seek funding for further work on approximate noise cancellation, as well as other possible applications which may include different physics, such as electrodynamics, and different formulations of the boundary-value problems, such as scattering.

It is our pleasure to acknowledge most useful discussions with Jan Hesthaven, Wu Li, Michael Overton and Victor Ryanben'kii.

Human/Robotic Exploration of the Solar System

Josip Lončarić and Manuel Salas

Exploration of the solar system will be most effective if both humans and robots are synergistically combined. Done correctly, this approach can reduce risks, improve efficiency, and accomplish goals faster. The challenge is to understand the ways in which this could be accomplished and how this mix might evolve over the next 10–40 years with the incorporation of revolutionary aerospace systems concepts. We have organized a workshop which brought together experts from academia, government, and industry to address these challenges.

This workshop, held on November 6–7, 2001, was aimed to support the development of a preliminary plan which would maximize the scientific return and enable the human exploration and development of space. The scope of this effort includes both planetary science and "in space" platform science applications beyond low Earth orbit. Specific objectives are: (1) identification of advanced revolutionary systems concepts, (2) identification of required technologies to enable these capabilities, (3) an evaluation of the evolution of the relative roles of humans and machines to implement these concepts, and (4) an identification of the science that would be enabled by these capabilities. Support for this project was provided by the Revolutionary Aerospace Systems Concepts (RASC) activity at NASA Langley. The workshop attracted 93 participants from government, academia and industry. After the workshop, session leaders gathered at ICASE on November 8th, 2001 to draft the final report. Moreover, the presentations and the NIAC RFI submissions were converted to PDF format and published on the workshop web site.

Additional visual illustrations of the exploration concepts presented at the workshop will be prepared by JF&A. The final NASA Conference Proceedings should be published in 2002.

This work is being conducted in collaboration with Robert Cassanova (NIAC) and Lewis Peach (USRA).

Aerodynamic Transonic Drag Prediction Using an Unstructured Multigrid Navier-Stokes Solver

Dimitri J. Mavriplis

The objective of this work is to assess the capability of an unstructured grid Navier-Stokes solver at predicting drag in the transonic cruise regime of a transport aircraft.

The flow over a wing-body transport aircraft configuration was computed on a grid of 1.6 million points and a grid of 13 million points at various Mach numbers and lift coefficient values. The results were compiled

as a series of drag polars and drag rise (drag versus Mach number at fixed lift coefficient) curves. A total of 72 individual cases were computed on the 1.6 million point grid, which was performed in about one week on the ICASE PC cluster using 16 to 32 processors. A total of six cases were computed on the 13 million point grid which was performed on the SGI NAS Origin 2000 machine using 64 to 128 processors. The drag results were found to be in relatively close agreement with results from other validated structured, unstructured, and overset grid method codes in the workshop, although a consistent bias in the lift at a given angle of attack existed between these numerical results and the experimental wind tunnel values. The ability to compute large numbers of cases with good accuracy on unstructured grids using inexpensive PC clusters was demonstrated through this exercise. Results from this study were presented at the 40th AIAA Aerospace Sciences Meeting in Reno, NV, January 2002.

More computations on additional grids are to be performed and the ability of adaptively generated meshes to reduce solution time and increase accuracy are also to be studied.

Investigation of Multigrid-implicit Higher-order Accurate Time-stepping Procedures for Unstructured Mesh Navier-Stokes Simulations

Dimitri J. Mavriplis and Giridhar Jothiprasad

The accurate solution of transient fluid flow problems as required in large eddy simulations, can become very cpu-time intensive due to the long simulation times required and large number of time steps employed. This work explores the feasibility of reducing the overall simulation time for a given level of accuracy by resorting to a smaller number of higher-order accurate time steps and using more efficient implicit solution techniques at each time step.

Based on the work of H. Bijl, M. Carpenter, and V. Vatsa, an implicit Runge-Kutta time stepping scheme has been implemented in an existing two-dimensional unstructured Navier-Stokes solver. A four-stage and a six-stage Runge-Kutta scheme are employed which are third-order and fourth-order accurate in time, respectively. Each stage of the Runge-Kutta schemes represents an implicit nonlinear problem which is solved using the agglomeration multigrid scheme previously developed for steady-state problems. This multigrid solver has also been used as a solver for a second-order backwards difference time stepping scheme. Design accuracy for both Runge-Kutta schemes has been demonstrated for laminar flow over a circular cylinder. A comparison of the time required to solve the nonlinear problem at each time step using a linear multigrid algorithm and a nonlinear multigrid algorithm has also been investigated. The linear multigrid algorithm has been found to be substantially faster than the nonlinear multigrid algorithm for this task.

The relative efficiencies for a given accuracy level of the various Runge-Kutta schemes and backwards differencing schemes solved with linear and nonlinear multigrid methods are to be compared. The effectiveness of using the multigrid solvers as preconditioners to a Newton-Krylov method is also under investigation. These results are to be presented at the AIAA Fluid Dynamics conference in June 2002.

Parameter-varying Gain-scheduled Fault Tolerance Control of an Aircraft

Jong-Yeob Shin

Recent aircraft flight control design research has concentrated on the development of control systems which stabilize an aircraft robustly and allow to recover aircraft performance under adverse conditions (actuator/sensor/engine failures and bad weather). One promising approach to designing robust Fault Tolerance Controller (FTC) for an aircraft under adverse conditions is use of linear parameter varying (LPV) control synthesis, since aircraft dynamics vary significantly according to angle of attack, velocity,

dynamic pressure, and so on. Aircraft dynamics can be described by a quasi-LPV model with scheduling parameters which are also states of the dynamics model.

To apply an LPV control synthesis to design a FTC, control component failure cases should be modeled as an LPV system. Usually, control surface failure cases are modeled as linear functions of fault parameters. The fault parameters should be measurable on-line to implement an LPV controller. We have currently used the optimal two-stage Kalman Filter to estimate fault parameters. In this case, the scheduling parameter is estimated with bounded uncertainty. We have formulated an LPV synthesis methodology with scheduling parameter uncertainties. The scheduling parameter uncertainties are represented as an uncertainty block in the LPV synthesis methodology. The designed LPV controller may lead a conservative result since the LPV synthesis methodology can not count on the uncertainty structure. In order to reduce conservatism of the controller, scaling factor S is introduced. The robust LPV controller problem is to find S and a controller K, which is not a linear matrix inequality problem. We have completed coding the robust LPV controller problem in MATLAB using an iteration method.

In future work, the robust LPV controller will be integrated with the fault parameter estimator. Also, a model of actuator failures will be considered as nonlinear functions of the fault parameter. Developing as reliable quasi-LPV model of an aircraft dynamics with fault parameters is still an open problem. The problem will be investigated based on research of a function substitution method.

This research is conducted in collaboration with Dr. Christine Belcastro (NASA Langley) and Prof. N. Eva Wu (Binghamton State University of New York).

Knowledge Discovery in Large Scale Distributed Data Sets with High- and Infinite-dimensional Data

Eduardo Socolovsky

To produce new approaches, algorithms, and tools to help extend the limits of computational feasibility and reduce the cost of performing clustering and dimension reduction on high-dimensional large-scale distributed data sets. Most presently used data analysis techniques become unfeasible or costly for very modest size data sets. The key factors to overcome this problem, are the computational efficiency of the algorithms, as well as the scalability of the algorithm and its implementation. Surveys indicate that between 70% and 80% of all data mining applications involve some form of clustering, which is a critical step in, e.g., statistical data analysis, pattern recognition, KDD, image processing, and data layout. Clustering high-dimensional data sets is a contemporary challenge. Dimension reduction is often crucial for high-dimensional data since, generally, the computational complexity grows exponentially with the dimension, and is also important as an analysis technique, such as Principal Component Analysis (PCA), also known as empirical orthogonal functions (EOF), Karhunen-Loeve transform, or normal modes.

In clustering a measure of similarity and/or a measure of density are used to detect groups or patterns in data. The most common is the Euclidean distance between data points, and the standard density is "number of points per unit volume." However, for high-dimensional data, the Euclidean distance does not work well, and the above density becomes useless since the required number of points grows exponentially with the dimension. For higher dimensional data and pattern recognition, clustering methods adopt more adequate measures of similarity, like Pearson's product-moment correlation or the cosine measure. An important problem with the above and other similarity measures in high dimensions is that, the triangle inequality doesn't hold. Among the results we have obtained, is a measure of dissimilarity strongly connected to the cosine measure that satisfies the triangle inequality. With the correlation similarity measure the bulk of the

computation and error propagation is in the dot-products, in particular the O(N) inner products required for the similarity measure matrix. We outlined new mixed agglomerative-partitioning algorithms that (at least in the average case) compute only O(N) inner products using our results on the two measures to generate approximate similarity and dissimilarity matrices (or equivalent bounds), that can be obtained from already computed inner products plus a few more floating point operations.

In PCA the set of variables or features are transformed into a new mutually uncorrelated (orthogonal) set of variables, and a smaller representative subset of variables is selected with a variance maximization criterion. Computationally, the transformation is obtained from the Singular Value Decomposition (SVD) of the matrix formed by the data points, and the new variables are given by the eigen-vectors corresponding to the largest singular values of the matrix. The original data is then projected onto the space spanned by the selected eigen-vectors. However, finding the SVD is computationally intensive and is a contemporary challenge to adapt for distributed data, which is resolved by adopting a PCA approximation. Furthermore, for some data sets the new variables are difficult to interpret and PCA does not provide a satisfactory representation, as frequently occurs with climate data sets. Often a representation in term of the original variables is preferred, hence as is done in Independent Component Analysis, we intend to investigate the use of other directions. The new directions are obtained or suggested by the results of clustering the original variables, thus obtaining a different matrix factorization. For scalability, current data mining system architectures favor a distributed agent approach to generate local components that are later merged into a global result, often based on a peer-to-peer agent collaboration and negotiation which can result in high communications demands. We will also explore Data Swarming, a non-traditional biologically inspired approach to software design and scientific applications in which the results emerge from the work of a collection of agents that perform simple tasks and communicate through a global medium.

Review of Fusion Propulsion for Spacecraft

Gerald Walberg

This work was carried out under the Revolutionary Aerospace Systems Concepts (RASC) program. Direction was received from NASA Headquarters to include fusion propulsion in the FY 2002 RASC studies. In order to address fusion propulsion in an informed manner, it was decided to carry out a literature survey of fusion research and of spacecraft designs using fusion propulsion in order to assess the current state of the art.

The literature surveyed consisted of recent (1980 to present) survey articles, research results, proposals for proof-of-concept investigations and published spacecraft designs. Both magnetic-confinement fusion and inertial-confinement fusion were addressed. It was found that a vast body of experimental and analytical research results exists and is sufficient to allow credible conceptual designs of fusion propulsion systems. When spacecraft are designed based on extrapolations of this currently existing database, they are very large (typical overall dimensions of 100–200m) and massive (6000–7000 metric tons), and require extensive in-space assembly. In order to achieve acceptably small and compact fusion propulsion systems, new approaches to fusion that have not yet been experimentally validated must be employed.

A RASC White Paper has been prepared and will be used to set the acceptable parameter space for the 2002 studies.

COMPUTER SCIENCE

Methods Of Separation Assurance For Instrument Approach Procedures

Maria Consiglio

A method to provide automated air traffic separation assurance services during approach to or departure from a non-radar, non-towered airport environment is investigated. The method is constrained by the current NAS infrastructure without radical changes or ambitious technology investments.

The proposed procedures are designed to grant access to a large number of airfields that currently have no or very limited access under Instrument Flight Rules (IFR) thus increasing mobility with minimal infrastructure investment. While mobility, defined as point to point transportation of people and goods may be increased total distance traveled and demand on busy airports may be reduced.

Following the definition of the procedures a simulation study is under way that models the ground-based airport automation to estimate the system behavior and response under given conditions. We completed coding the first release of the simulation driver and sequencing algorithm. We are currently doing testing and validation and verification of simulation results.

This work is done in collaboration with Sheila Conway (NASA Langley).

Analysis of Causal Event Relationships in a Distributed Air Traffic Management Simulation

Maria Consiglio

Understanding the behavior of a parallel, distributed system can, among other things, lead to more efficient implementations. Distributed systems implementations that assume a global clock are often simpler to implement and easier to understand. Potential inconsistencies and deadlock conditions due to the inherent non-determinism of a distributed computation are prevented as the computation proceeds time stepping, synchronizing at every tick of the global clock. An alternative approach allows distributed components of the simulation to use their local clocks while ensuring event ordering as imposed by the causality constraints. Conservative and optimistic (time-warp) implementation methods can be used once the system behavior has been fully characterized.

Identifying the causal and temporal relationships can eliminate the need of an artificially imposed global time which can introduce unnecessary communication overhead, reduce the degree of parallelism, limit the scalability of the system, and compromise the validity of the computation.

In this work, the causal and temporal event dependencies in a distributed air traffic simulation (FFSim) are analyzed to verify the viability of a distributed time implementation that ensures correct results and satisfies repeatability requirements. FFSim (Free Flight Simulation) is a workstation-based, medium fidelity air traffic simulation designed to test DAG-TM (Distributed Air/Ground Traffic Management) operational concepts that is being developed in the Air Traffic Operations Laboratory (ATOL) at NASA Langley Research Center.

This work is done in collaboration with Sheila Conway (NASA Langley).

Tidewater Research Grid Project (TRGP)

Thomas M. Eidson and Josip Loncaric

A recent trend in scientific computing has been the increased use of Grid computing. Grid computing is defined as the development and execution of distributed applications across wide-area networks where administrative and security issues are non-trivial. Very high-performance computers have become increasingly

expensive and researchers are looking to the use of large numbers of lower-performance machines to meet their computational needs. Unfortunately, these machines are located at various locations where the Internet (or an internet) is involved, thus the need for Grid computing. A number of projects around the world are focusing on the technology and security of remote job execution, few are looking at the security issues involved with managing a distributed user base located at multiple sites. TRGP was formed to assist ICASE and other related organizations in learning Grid software basic technology and to provide a base platform for the development of Grid programming environments. Additionally, the user-management security/trust issues are being studied.

The current focus of the project has had two objectives. The first was to use currently available software to implement a Grid infrastructure. The Globus Toolkit was used to provide the distributed computing functionality. This includes remote process management, file transfer capability, message passing and other signaling, and security. The PGP system was used to add secure person-to-person communication since the participants in TRGP will be located at separated sites. These packages have been installed and a set of Perl scripts were written to provide a simple and consistent interface for TRGP users. This has been all documented via Web pages. The goal being that both system administrators and users will have single clear source to learn about TRGP and Grid computing. The second objective was to recruit organizations to part of TRGP. A workshop was held to present the above TRGP system to potential organizations. Representatives from Old Dominion University, Jefferson Labs, and William and Mary were invited. The response was favorable as all have expressed interested in joining TRGP.

In the next phase of this project we have three objectives. The first will be to give installation support to any organization that wishes to join TRGP. While the goal of the TRGP documentation and software is to be self-sufficient, it will be important to get feedback from early users to improve the documentation and software. The second objective will be to work with users to develop Grid applications. The large number of parallel applications designed for homogeneous parallel architectures do not necessarily port to Grid architectures. Applications will need to have a heterogeneous nature to map to the heterogeneous collection of machines and networks. One way this can be done is to try new algorithms. However, a more fruitful approach may be to develop more complex, integrated applications. This can be done by coupling data analysis to an existing application so that application can be interactively monitored and possibly steered. Another approach is to develop applications that solve more complex problems and involve multiple types of physics. Multi-dimensional optimization is one example of this type of application. The final approach in this phase will be to study the Globus Toolkit and relating programming techniques. The objective will be to become familiar with any new heterogeneous, distributed programming techniques to provide the best assistance to TRGP users.

15th International Conference on Theorem Proving in Higher Order Logics (TPHOLs 2002)

César Muñoz and Hanne Gottliebsen

Theorem proving technology is currently being used in industry and government in places such as Intel, Rockwell-Collins, Honeywell Aerospace, NASA Langley Research Center, NASA Ames Research Center, and the Naval Research Laboratory. Several universities in the United States and around the world also have an active formal methods research program to include theorem proving and applications. Industrial usage and increase in system complexities are placing new demands on theorem proving, such as improved automation, domain specific theories, and interoperability of multiple verification tools. For technology transfer to succeed, theorem proving researchers need to understand these new demands and create new

research thrusts to address the issues.

TPHOLs is the premier conference on the theory, development, and application of higher order logic and theorem proving. The conference brings together international experts from government, industry, and academia for four days of research presentations, work-in-progress presentations, discussions, and demonstrations. In 2001, ICASE, NASA Langley, and Concordia University put together a bid to host the 15th edition of this prestigious conference on August 20–23, 2002 in Hampton, VA. The bid was chosen in a voting process by the majority of the TPHOLs community. Since then, the TPHOLs 2002 organizing committee has customized and improved the START Conference Manager Web Server to support: electronic paper submissions and registrations; and web-based reviewing of submitted works and voting for the selection of the TPHOLs 2003 site.

The 15th edition of TPHOLs will be co-located with the First Workshop on Formalizing Continuous Mathematics. More than 60 researchers in the area of theorem proving and higher-order logics are expected to attend both meetings. The proceedings of the conference will be published in the Springer-Verlag's Lecture Notes in Computer Science series.

The conference and workshop are being organized with the collaboration of Víctor Carreño (NASA Langley), Sofiéne Tahar (Concordia University), and Andrew Adams (University of Reading).

Fundamental Algorithms for the En-route Phase of DAG-TM

César Muñoz, Alfons Geser, and Hanne Gottliebsen

Free-Flight is a new concept for air traffic management. Under free-flight rules, air traffic separation is distributed among the actors of the aerospace system. DAG-TM is the NASA implementation of the Free-Flight concept. It consists of a set of *elements*, also called *Concept Elements*, each one of which addresses a particular phase of a flight. Concept element 5 corresponds to the en-route phase. The main problem in this phase is the avoidance of air traffic conflicts. The objective of this work is to develop a set of formally verified algorithms for the en-route phase of DAG-TM. Formal verification will substantially increase safety of the increasingly autonomous and complex new air traffic management systems.

In the past, we have successfully applied formal methods techniques to design a three-dimensional algorithm for tactical conflict resolution (KB3D) and strategic conflict resolution and recovery (RR3D). In this work, we have extracted and modified the conflict detection algorithm in KB3D towards an algorithm, CD3D, that is not only correct but also complete. We have so developed a suite of fundamental algorithms for the en-route phase of free flight that includes:

- CD3D: A *correct* and *complete* three-dimensional conflict detection algorithm.
- RR3D: A strategic algorithm for conflict resolution and recovery that is based on geometry.
- KB3D: A *correct*, improved version of the original conflict resolution algorithm.

The RR3D algorithm has significantly improved and matured. Its current version and a mathematical argument for its correctness are documented in an ICASE Technical Report. We established two theorems that we believe represent a breakthrough in our attempt to prove correctness of RR3D. All three algorithms have been analyzed using rigorous mathematical techniques. Furthermore, CD3D and KB3D have been mechanically verified in the PVS system. Prototype implementation of the algorithms are available through the Internet and simulations on high-density free-flight scenarios are being performed.

Formal methods are a promising technology for safety of avionics systems. We will continue the development of fundamental algorithms for other phases of DAG-TM using formal methods techniques. In particular, we are beginning to study the merging and self-separation problems of Concept Element 11

(Terminal Area).

This work was done in collaboration with Gilles Dowek (INRIA) and Florent Kirchner (ENAC).

A Formal Verification of the SPIDER Diagnosis Protocol

Alfons Geser

SPIDER (Scalable Processor-Independent Design for Electromagnetic Resilience) is a case study for the Federal Aviation Agency that shall demonstrate the feasibility of Formal Methods for the certification of safety-critical hardware according to document DO-254. It shall provide feedback on problem areas and shall serve as material for DO-254 training.

SPIDER is composed of a number of Processing Elements (PEs) that are connected via the Reliable Optical Bus (ROBUS). The ROBUS consists of two columns of nodes, the BIUs and the RMUs, which are connected to each other but not connected among their own kind. The nodes are fault-containment units, i.e., all nodes fail independently. Nodes may exhibit various kinds of faulty behavior, including two-faced, malicious behavior. To counteract the danger that emergence of faults confuses the system, each node maintains and collects evidence about the health status of other nodes through direct and indirect observations. The purpose of the Diagnosis Protocol is to distribute each node's knowledge about the health status reliably, and to form convictions, i.e., correct claims of a node being faulty that all good nodes share. Diagnosis works only if enough hardware is good (Maximum Fault Assumption, MFA) and the health status information is intact (Correct Active Sources). Having finished the correctness proof in PVS at the start of the period, our primary goal was to simplify and to document the proof. Opportunities to migrate to a dynamic readmission of transiently failed nodes were discussed. During this discussion a previously neglected important point came up: can we prove that diagnosis strictly increases the reliability of the ROBUS? We found that for this purpose the MFA has to be weakened such that only undeclared nodes are counted. This dynamic MFA does indeed profit from convictions as can easily be shown. The Diagnosis Protocol, the Interactive Consistency Protocol, and the correctness proofs of the two needed a few essential changes to accomodate the dynamic MFA. We have implemented these design changes, including the correctness proofs, and are now about to write an ICASE Technical Report.

In the near future we plan to start designing a Readmission Protocol that allows formerly faulty but recovering nodes to be reconsidered as good nodes.

This work was done in collaboration with Paul S. Miner (ATM, NASA Langley).

FLUID MECHANICS

Seedless Laser Velocimetry with Laser-induced Thermal Acoustics

Roger Hart

Non-intrusive measurement of flow velocity by various laser-based methods provides information of great significance to the experimental fluid dynamics community. However, the only methods to have achieved widespread use to date are laser doppler velocimetry and particle interval velocimetry, both of which require the flow to be seeded with small ($\tilde{1}$ micron) particles to serve as light scatterers. Seeding is not feasible in some wind tunnels due to concerns over removal of spent seed, clogging of flow straightening screens, or abrasion of finely polished surfaces. Additionally, there are regions in air flows of interest, such as vortex cores over delta wings or in recirculation regions behind rearward facing steps or leading-edge slats, where useful seed concentrations may be difficult or impossible to achieve. There is, thus, considerable interest in a laser velocimetry technique that can provide the dependability, ease of use, and quality of data of existing methods without seeding. Laser-induced thermal acoustics (LITA) is a relatively new technique which has great promise as a robust, reliable seedless laser velocimetry method. Our objective is to further develop the theoretical and technical basis for LITA velocimetry in the laboratory, and to demonstrate the utility of LITA velocimetry through a variety of 'real-world' wind tunnel measurements at NASA Langley.

Considerable theoretical and laboratory evaluation of LITA velocimetry has already been accomplished, although work continues in support of the improvement of our designs for fieldable measurement systems. Our overall design philosophy springs from the realization that a system must be relatively easy to install and use and must reliably produce dependable data; a system that does not meet these requirements will be of no interest to our user community. To that end our designs stress modularity, easy transport and installation, and the use of compact, turn-key laser systems. Of great significance as regards stability and accuracy is our use of a novel grating-based quadrature demodulation technique (invented by us). The current reporting period has been devoted to the completion of a two velocity component LITA velocimeter incorporating lessons learned from our earlier one-component prototype. The new instrument is fully remotely operable from a wind tunnel control room, and should be significantly more stable than the earlier version.

We are currently scheduled to conduct a demonstration of the new velocimeter at BART beginning in early May 2002 in which we will make velocity measurements of the flow above a high-lift wing. Our data will be compared with existing PIV data sets for that configuration. In February 2003 we will begin our first demonstration of supersonic LITA velocimetry at PCT, investigating the flow around a diamond-shaped model at free stream velocities ranging from transonic to Mach 3.5. The possible application of LITA velocimetry to the high-pressure exhaust flow from a (leftover) NASP model at 15" Mach 6 is under discussion.

This work is pursued in collaboration with R.J. Balla and G.C. Herring (AMDB, NASA Langley).

Time Accuracy of Large Eddy Simulation for Unsteady Flows

Guowei He

The objective of this research is to develop subgrid scale (SGS) modeling for Large Eddy Simulation (LES) of unsteady flows. The previous research has focused on the ability of LES on single-time flow properties such as energy spectrum. Attention has never been paid on the two-time or frequency energy spectrum. In fact, the frequency spectrum has wide application to unsteady flows. For example, the frequency spectrum

of velocity fluctuations determines the frequency distribution of far-field acoustic energy in aeroacoustics; the frequency content of turbulent energy characterizes the turbulent disturbance environment for receptivity; the noise reduction, synthetic jets, and coherent structure in flow control are associated with frequency energy spectrum.

We have shown that the eddy viscosity SGS models over-predict the two-time energy spectrum. The over-prediction could be very significant. Further, the necessary conditions for SGS models to correctly predict time correlation are derived. These conditions are used to investigate SGS models and suggest that the random forcing model and Lagrange dynamical model are recommendable for the two-time energy spectrum. They also indicate that the coefficients in the eddy viscosity SGS models should be history-dependent. We have developed a new two-parameter model and sub-Gaussian model for the two time energy spectrum. The former is constructed by the "sweeping" and "oscillation" parameters and the latter by the mean velocity of sub-Gaussianality.

Our future work will develop the Langevin-type and Lagrange dynamical SGS models for time accuracy of LES in unsteady flows.

This work is performed in collaboration with R. Rubinstein (NASA Langley).

Uncertainty in Computational Fluid Dynamics
Guowei He

The objective of this research is to develop a statistical approach to uncertainty in Computational Fluid Dynamics (CFD). We focus on the errors of CFD induced by either turbulence modeling or uncertainty in physical models. The motivation of this research is that NASA needs credible CFD simulations and aerodynamical optimization needs the quantification of uncertainty in CFD as input parameters.

We are developing the mapping closure approximation to quantify the uncertainty propagation. The mapping relates the random inputs and outputs in deterministic fashion. Actually, the truncated mapping has been used to calculate the first and second order moments in sensitive analysis. The demonstration cases are the passive scalars in shear flow and reactive scalars in random Gaussian flows. The probability density function, conditional dissipation rate, and conditional Laplacian are calculated and are in good agreement with direct numerical simulation. It is shown that the approach is able to describe the propagation of uncertainty in physical models. Two ICASE reports on this topic have been finished.

Our future work will apply the mapping closure approximation approach to the quasi-one-dimensional Euler CFD.

Multiple-relaxation-time Lattice Boltzmann Models in Three Dimensions
Li-Shi Luo

The simplest lattice Boltzmann equation (LBE) is the lattice Bhatnagar-Gross-Krook (BGK) equation, based on a single-relaxation-time approximation. Due to its extreme simplicity, the lattice BGK (LBGK) equation has become the most popular lattice Boltzmann model in spite of its well known deficiencies, such as the instability at low viscosity.

We have constructed two three-dimensional LBE models with 15 and 19 velocities based on the multiple-relaxation-time (MRT) lattice Boltzmann equation. The MRT LBE model (also referred to as the generalized lattice Boltzmann equation (GLBE) or the moment method) overcomes some obvious defects of the LBGK model, such as fixed Prandtl number ($\mathrm{Pr} = 1$ for the BGK model) and fixed ratio between the kinematic and bulk viscosities. The MRT lattice Boltzmann equation has been persistently pursued, and much progress has

been made in the following areas: formulation of optimal boundary conditions, interface conditions in multiphase flows and free surfaces, thermal and viscoelastic models, models with reduced lattice symmetries, and improvement of numerical stability. It should be stressed that most of the above results cannot be obtained with the LBGK models. Applying optimization techniques in coding, the computational efficiency of the RLBE method can be fairly close to that of the LBGK method for most practical applications (RLBE schemes could be *ca.* 15% slower than their LBGK counterparts in terms of the number of sites updated per second). Recently it was shown that the multiple-relaxation-time LBE models are much more stable than their LBGK counterparts, because the different relaxation times can be individually tuned to achieve 'optimal' stability.

The present work is a result of collaboration with D. d'Humières (École Normale Supérieure, France), I. Ginzburg (Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Germany), M. Krafczyk (Technische Universität Braunschweig, Germany), and P. Lallemand (Laboratoire ASCI-CNRS, Université Paris-Sud (Paris XI Orsay), France). The present work has been partially funded by the United States Air Force Office for Scientific Research under Grant No. F49620-01-1-0142 (technical monitor: J. Tishkoff).

We intend to apply the LBE MRT model for DNS and LES simulations.

STRUCTURES AND MATERIALS

Wholly Aromatic Ether-imide Liquid Crystals I. Synthesis and Characterization

Theo Dingemans

In order to improve the processability of single-wall and multi-wall carbon nanotubes, we have synthesized a series of wholly aromatic ether-imide model compounds composed of an electron-poor imide core and electron-rich aryl-ether flexible tails. We choose to work with this class of compounds because aromatic imides are able to form charge transfer complexes with closed-shell carbon nanostructures, and this interaction can be utilized to solubilize carbon nanostructures.

To date we have synthesized and characterized a novel series of low-molar-mass ether-imide rod-shaped model compounds. All ether-imides were obtained by terminating the appropriate rigid core dianhydride, i.e., pyromellitic dianhydride (PMDA), 1,4,5,8-napthalenetetracarboxylic dianhydride (NDA), 3,3',4,4'-biphenyl-tetracarboxylic dianhydride (BPDA), and 3,3',4,4'-oxydiphthalic dianhydride (ODPA) with three different flexible aryl-ether tails. The mono-functional aryl-ether amines, i.e., 4-(3-phenoxy-phenoxy)-phenylamine and 4-(3-phenoxy-3-phenoxy-phenoxy)-phenylamine, were synthesized using standard fluoro-displacement and Ullmann condensation techniques. The corresponding ether-imide model compounds were obtained in high yields using a one-step solution imidization procedure. Increasing the number of *meta*-substituted aryl-ether units reduces the melt transition temperatures and at the same time it increases the solubility of the model compounds. Most model compounds are crystalline solids and form isotropic melts upon heating. 2,7-Bis-(4-phenoxy-phenyl)benzo[*lmn*][3,8]phenanthroline-1,3,6,8-tetraone, however, displays a smectic A and rectangular columnar phase when cooled from the isotropic phase. This is the first example to date, in which a mesophase is detected in a wholly aromatic ether-imide compound. Increasing the number of flexible *meta*-substituted aryl-ethers results in low melting ether-imides that super-cool and form amorphous glasses with well defined glass-transition temperatures.

Future work will include temperature-dependent NMR, Raman spectroscopy, and atomic force microscopy (AFM) experiments, which will allow us to monitor and quantify the interactions between the model compounds and carbon nanotubes. In addition, we will use molecular modeling as a tool to predict which imide model compounds are the most promising candidates for forming charge transfer complexes with carbon nanotubes.

This research was conducted in collaboration with Kris Wise and Cheol Park (ICASE), and Peter Lillehei (NASA Langley).

Carbon Nanotube Pullout from a Polymer Matrix in a Nanocomposite

Sarah-Jane V. Frankland and Vasyl Michael Harik

Carbon nanotubes have been proposed as fillers to reinforce polymer matrices. The ability to transfer load across the polymer-nanotube interface is fundamental to the mechanical performance of these materials. To characterize the nanotube-polymer interfacial properties, a detailed theoretical study of the nanotube pullout from polymer matrices is being carried out. The deformation processes occurring in the composite as the nanotube moves within the matrix are relevant to the design and fabrication of polymer-nanotube composites as well as interfacial failure mechanisms. The objective of this study is to use atomic-level information from molecular dynamics simulation to identify deformation processes during pullout, to parameterize the related shearing behavior from the simulations, and to develop higher-level models that incorporate the simulated input.

Molecular dynamics simulations have been carried out for the process of a nanotube pullout from a crystalline polyethylene matrix. Semi-periodic variations in the nanotube velocity are observed which can be related to the local structure of a nanotube. Analysis of the force-velocity dependence has led to being able to fit the simulation data into a model. This model gives an estimate of the local effective viscosity. In this way, the shearing deformation of a nanotube-polymer nanocomposite may be evaluated.

Simulation data will be generated for non-bonded and chemically functionalized polymer-nanotube composites to further identify and model processes during nanotube pullout. Analogous viscosity information will be generated for and applied to the slippage of carbon nanotubes within a bundle in the design of woven nanotube fibers.

This work was done in collaboration with J.A. Hinkley and T.S. Gates (NASA Langley).

Transverse Moduli of Carbon Nanotube Ropes

Sarah-Jane V. Frankland

Single-walled carbon nanotubes occur in hexagonal packed bundles or ropes. The mechanical properties of these bundles as groups of nanotubes rather than individual nanotubes is not well-characterized empirically or theoretically. In particular, the transverse properties which depend on the weak non-bonding van der Waals interactions between the nanotubes have been generally ignored in favor of the more impressive longitudinal properties of perfect carbon nanotubes such as the Young's modulus typically reported to be 1 TPa. The transverse properties must be considered in the design of polymer composites or other materials such as woven nanotube yarns, which depend on nanotubes for reinforcement. The objective here is therefore to assist the design effort of these materials by providing reasonable computational estimates of the transverse moduli of carbon nanotube bundles.

In this work, the transverse moduli of carbon nanotube bundles have been calculated from a simple molecular statics model of rigid hexagonally packed nanotubes about 1 nm each in diameter. The intertube potential depends solely upon the van der Waals interactions between the nanotubes which are represented by the Lennard-Jones potential. The rigid approximation is reasonable for nanotubes of this size. Calculations have been done for the elastic constants C22, E22, bulk modulus K23, Poisson's ratio v23, and shear modulus G23, where 2 and 3 are the directions transverse to the nanotube axis. These independently determined values relate consistently via the Hashin relations. Comparisons were made with existing data in the literature. These calculations provide an estimate for the transverse behavior of nanotube bundles based on relatively simple consideration of van der Waals interactions.

This work will be extended to the calculation of other mechanical properties for additional nanotube ropes. Refinement of the nanotube-nanotube interaction potential is being considered. The moduli will be used in designing and evaluating the mechanical properties of nanotube yarns and polymer composites.

This work was done in collaboration with J.A. Hinkley, T.S. Gates, and E. Saether (NASA Langley) and R.B. Pipes (University of Akron).

Mechanics of Carbon Nanotubes

Vasyl Michael Harik

Carbon nanotubes possess extraordinary physical properties (e.g., high stiffness and strength along with enormous electrical and thermal conductivities). Potential applications range from new electronic devices and nanotube-based scanning probes to multifunctional polymer films and sensors for new aerospace structures. The goal of this research is to develop constitutive models for carbon nanotubes and a methodology for the implementation of continuum models at the nanometer scale.

Ranges of validity and length-scale limitations of the continuum models for carbon nanotubes under compressive loads are examined. Hierarchical dimensional analysis of the nanomechanical buckling problem and the geometric and material parameters involved is carried out. As a result, three classes of carbon nanotubes are identified. One of the classes consists of the newly predicted carbon nanobeams. The scaling laws and the key non-dimensional parameters controlling the deformation process of nanotubes have been derived. Expressions for critical strains are tailored for various nanotubes and their values are compared with the molecular dynamics simulations. Model applicability maps are constructed for different nanotube geometries in the parameter space.

Future research involves analysis of the nanotube-based AFM tips and the effects of nanotube geometry on the constitutive properties of nano-structured materials. Applicability of advanced shell theories will be examined as well.

This research is conducted in collaboration with T.S. Gates, M.P. Nemeth, and D.R. Ambur (MDB, NASA Langley).

Modeling of Multifunctional Composite Materials

Vasyl Michael Harik

Design of new aerospace structures, such as flexible wings, structures with active controls, multifunctional membranes, and inflatable antennas require fundamental understanding of electromechanical coupling in material behavior so that they can be modeled accurately in structural analyses. Nanostructured materials offer additional benefits that stem from their superior physical properties. The goal of this research is to develop hierarchical constitutive models that link the nano-scale molecular structures with continuum micromechanics. Such models are critical for the development, design, and optimization of novel nanocomposites.

Constitutive models for multiphysics phenomena are examined along with the structure of carbon-filled polymer matrix systems. Homogenization criteria for hierarchical connectivity and thermodynamically consistent material averaging are derived for nanotube-reinforced polymer composite systems. This modeling approach has been used to link molecular dynamics simulations of nanocomposites with nanomechanical models that are analogous to similar models in micromechanics.

The future work is directed toward a better understanding of applicability and limitations of this methodology and alternative techniques for multi-scale modeling.

This research is carried out in collaboration with S.J.V. Frankland (ICASE), D.R. Ambur and T.S. Gates (MDB, NASA Langley).

Stitched Stiffened Panels Loaded in Shear

Navin Jaunky

Progressive failure studies of composite panels were carried out for stiffened stitched panels. These studies were carried out to validate modeling methodologies for intralaminar damage modes being developed. The development of such damage modeling methodologies are discussed in earlier reports.

Intralaminar damage modes such as matrix cracking, fiber-matrix shear, and fiber failure are modeled by degrading the material properties. The stitched panels were stiffened panels and were loaded in in-plane shear. Two stiffened panels were considered, one had a notched and the other was un-notched. These panels were loaded well into their postbuckling regime. Experimental results from the test include strain field data from video image correlation in three dimensions (VIC-3D) in addition to other strain and displacement

measurements. Progressive failure analyses of these panels did not include interlaminar damage mode since the panels are stitched. Initial geometric imperfections and thickness imperfections were included in the finite element models. The three intralaminar failure modes considered for the stitched panels in the study accurately represent the damage scenario in the postbuckling regime. The analytically determined panel response, failure modes, and damage locations compare well with the experimental results for the pointwise as well as for full field measurements. Including thickness imperfection provides better agreement with the experimental results. Progressive failure analyses results with successive loading and unloading sequences to mimic the experimental loading conditions are also in good agreement with the experimental results. It was found that these progressive failure analyses can account for the damage accumulated in a previous run. Damage detection after failure was attempted on the un-notched panel using a thermographic scan.

Future work will focus on more comparison of progressive failure analyses for different types of loading. Damage detection at different load levels during the experiments will be attempted using thermographic scan. Full field measurement using VIC-3D will also be used. Attempt to incorporate physics based failure criteria in the progressive failure analyses will be made.

This work is done in collaboration with Damodar R. Ambur and Mark W. Hilburger (NASA Langley).

Intralaminar and Interlaminar Progressive Failure Analyses

Navin Jaunky

A progressive failure methodology is developed that includes the interaction of intralaminar and interlaminar damage modes. The intralaminar failure is as described above. The interlaminar failure mechanism such as delamination is simulated by positioning interface elements between adjacent sublaminates. A non-linear constitutive law is postulated for the interface element that accounts for a multi-axial stress criteria to detect the initiation of delamination, a mixed-mode fracture criteria for delamination progression, and a damage parameter to prevent restoration of a previous cohesive state. The methodology is validated using experimental data available in the literature on the response and failure of quasi-isotropic panels with centrally located circular cutouts loaded into the postbuckling regime.

Very good agreement between the progressive failure analyses and the experimental results is achieved if the failure analyses includes the interaction of intralaminar and interlaminar failures. The analyses demonstrated the following;

1. The intralaminar damage induced the initiation of delamination at the free edge of the cutout at the same locations identified in the experiments.
2. Delamination growth occurred perpendicular to the loading direction in regions where large compressive loads were present.
3. Catastrophic failure was a consequence rapid delamination growth.
4. Delamination growth followed by delamination arrest leads to a residual strength, a finding consistent with the experimental data. After further loading, delamination growth occurs leading leading to catastrophic failure.

Future work will focus on more comparisons of progressive failure analyses for different types of loading. Damage detection at different load levels during the experiments will be attempted using thermographic scan. Full field measurement using VIC-3D will also be used. Attempt to incorporate physics based failure criteria in the progressive failure analyses will be made.

This work is done in collaboration with Vinay Goyal and Eric Johnson (Virginia Polytechnic Institute and State University). Damodar R. Ambur (NASA Langley) was also involved.

Debonding in Stringer Reinforced Composite Components
Ronald Krueger

Many composite components in aerospace structures are made of flat or curved panels with co-cured or adhesively bonded frames and stiffeners. Previous investigations of the failure of secondary-bonded structures focused on loading conditions typically experienced by aircraft crown fuselage panels. First tests were conducted with specimens cut from a full-size panel to verify the integrity of the bondline between the skin and the flange or frame. A simpler and cheaper specimen configuration that would allow detailed observations of the failure mechanism at the skin/flange interface was proposed later. The investigations focused on the failure mechanisms of a bonded skin/flange coupon configuration subjected to tension, three and four-point bending, and combined tension/bending loading. The failure that initiates at the tip of the flange in these specimens is identical to the failure observed in the full-scale panels and the frame pull-off specimens. An analytical methodology was developed to predict the location and orientation of the first transverse matrix crack based on the principal transverse tension stress distribution in the off axis plies nearest the bondline in the vicinity of the flange tip. A fracture mechanics approach was used to investigate delamination onset once the initial crack had formed. The initial crack was modeled as a discrete discontinuity at a location suggested by the microscopic investigation. The complex nature of the failure observed during the experiments, where the delamination changed across the specimen width from a delamination running at the skin surface 45°/-45° layer interface to a delamination propagating in the bondline above, suggests the need for a three-dimensional model. Since many layers of brick elements through the thickness would be required to model the individual plies, the size of three-dimensional finite element models, however, may become prohibitively large. Two-dimensional models of a longitudinal cut through the specimen allow for a detailed modeling of the individual plies and the adhesive in thickness direction. Two-dimensional models are preferred by industry due to the fact that modeling time, as well as computational time, remains affordable, especially if many different configurations have to be analyzed during the initial design phase. However, it is inherent to any two-dimensional finite element model that the geometry, boundary conditions, and other properties are constant across the entire width. The effect of two-dimensional modeling assumptions is most marked for 45° plies because of their high in-plane Poisson's ratio, while it is small for 0° and 90°. The objective of the current study was to evaluate how the results obtained from two-dimensional finite element models of the specimen compared to data obtained from full three-dimensional simulations in order to find the limitations of using simple two-dimensional models. Investigating the limits and usefulness of any numerical model is in general an important engineering science problem that reaches beyond the current analysis of the skin/stringer debond specimen.

Finite Element analyses were performed for simple skin/flange specimens subjected to tension and bending loads. Geometrically nonlinear finite element analyses using two-dimensional plane-stress and plane-strain elements as well as three different generalized plane strain type approaches were performed. The computed skin and flange strains, transverse tensile stresses and energy release rates were compared to results obtained from three-dimensional simulations. The plane stress and plane strain models provided results for skin and flange strains, as well as energy release rates, which form an upper and lower bound of the results obtained from full three-dimensional analysis. The results from generalized plane strain models fall between the results obtained from plane stress and plane strain models. The generalized plane strain models capture the surface strains on the flange and skin very well. Computed energy release rates are within 9% of the results from three-dimensional analysis, however, there is not consistency across the load cases with respect to which model performs best. Stresses obtained from plane strain and generalized plane

strain models, were excessively high when compared to results from three-dimensional analysis. The stresses from full three-dimensional analysis were lower than results from any of the two-dimensional models, but are closest to the plane stress results. Based on the results of this investigation it is recommended to use results from plane stress and plane strain models as upper and lower bounds. Two-dimensional models may also be used to qualitatively evaluate the stress distribution in a ply and the variation of energy release rates and mixed mode ratios with delamination length. The current recommendations are based on the analysis of the skin/stringer specimen with a particular layup. Further analyses are required before the recommendations may be generalized.

The current study presents an intermediate step where three-dimensional models were created by extruding two-dimensional models across the width. The fact that the delamination changed across the specimen width from a delamination running at the skin surface 45°/-45° layer interface to a delamination propagating in the bondline above, however, is still not accounted for in this model. Nevertheless, the three-dimensional model takes width effects into account and therefore provides insight into the limitations of the use of two-dimensional finite element models. For future detailed modeling and analysis of the damage observed during the experiments, the shell/3D modeling technique offers great potential for saving modeling and computational effort because only a relatively small section in the vicinity of the delamination front needs to be modeled with solid elements.

This work is done in collaboration with Isabelle L. Paris (National Research Council), T. Kevin O'Brien (Army Research Laboratory, Vehicle Technology Directorate located at NASA Langley), and Pierre J. Minguet (The Boeing Company, Philadelphia).

Intelligent Optics

Mark Little

Intelligent optics, materials, or devices whose optical properties may be controlled by external means, have a significant role in many areas of today's society. Some include the communications industry, scientific research, and space applications. One problem with current intelligent optical materials is a characteristically slow response time. For use in communications and space it is imperative to have fast optical devices. One possible solution is to exploit the Stark and Zeeman effects in materials. These quantum mechanical lifting of electronic degeneracy by electric or magnetic fields may induce a change in the materials optical properties that can be exploited. Since these transitions are quantum in nature their response times will be very fast. In addition, current optics are designed to work at a set frequency range. If materials could be developed that would allow the frequency range of standard optical devices to be changed without the need to continually change components, the optics world would be revolutionized. The goal of this research is to fabricate new optical thin film (OTF) materials that use the Stark, Zeeman, or other effects as its active optical 'switch'.

Current work is focused on the exploration growth for new OTF materials. The growth systems for the lab have been installed and are producing products. The Stark and Zeeman effect will require an atomically isolated dopant level residing in a host material. Many dopant candidates are being tried and the optical properties with applied fields are being measured. Various host materials, including standard optical glasses, oxides, wide band gap semiconductors (both crystalline and amorphous), and ferroelectric materials are being investigated. In addition to the optical characterization, basic electronic testing capabilities of these materials have been established to check their suitability as new electronic materials.

Future work is to include the continued growth and characterization of new materials for smart optical devices based on the Stark and Zeeman effects. Also new methods for creating active diffraction gratings are

in the infancy stage. Brainstorming is occurring to determine a feasible method of achieving this goal. There is interest in this area of research from the Army Office of Research and a collaborative effort is attempting to be established. I would like to thank Glen King and Sang Choi for their help and guidance with this research.

Constitutive Modeling of Nanotube/Polymer Composites

Gregory Odegard

In the last few years, SWNT-reinforced polymer composites have generated considerable interest in the materials research community partly because of the potential for large increases in strength and stiffness when compared to typical carbon-fiber-reinforced polymer composites. In order to facilitate the development of nanotube-reinforced polymer composites, constitutive relationships must be developed to predict the bulk mechanical properties of the composite as a function of molecular structure and bonding of the polymer, the nanotube, and the polymer/nanotube interface.

A modeling methodology has been developed that predicts continuum mechanics-based elastic constants of nanotube composites using atomic-scale information. Molecular structure and bonding information, which is obtained through Molecular Dynamics simulations, is used to construct an equivalent-continuum model of a nanometer- scaled representative volume element of the nanotube composite. Specifically, models have been generated for nanotube/polyimide and nanotube/Polypropylene composites (both with a PmPV interface). It has been shown that the predicted elastic properties agree with other multi-scale modeling methodologies and with experimental results. Therefore, the model is ready to be implemented as a tool in the development of nanotube/polymer composites.

Future work will involve the modeling of additional nanotube composite systems. In order to understand the effect that covalent bonding between the nanotube and polymer has on the overall mechanical properties of the composite, functionalized and non-functionalized nanotube/polyethylene composites will be modeled. Nanotube/liquid crystal polymer systems will be modeled to explore their potential use as structural materials.

This research has been performed in collaboration with T.S. Gates, E.J. Siochi (NASA Langley), S.J.V. Frankland, V.M. Harik, C. Park, K.E. Wise (ICASE), R.B. Pipes (University of Akron), and P. Hubert (Old Dominion University).

Nanoindentation of Nano-structured Materials

Gregory Odegard

Nanoindentation is a promising method of measuring mechanical properties of materials at the nanometer-length scale. Among the advantages of nanoindentation is the ability to examine surface effects and individual constituents of a structural material. Because nanoindentation has been used almost exclusively for metallic and ceramic materials, its application to characterizing viscoelastic properties of nano-structured polymers and polymer composites needs to be explored in detail.

A series of tests has been performed on various advanced structural polymers for measurement of viscoelastic properties. The dependence of measured properties on testing parameters (e.g., strain rate, harmonic displacement, and harmonic frequency) has been investigated. Procedures for mounting bulk samples and thin films have been developed. Comparisons of measured viscoelastic properties obtained from other test methods show remarkable agreement. Together, these studies have established an overall testing procedure that can be used for testing a wide range of polymers under various test conditions.

Future work will involve the viscoelastic characterization of nanotube/polymer composite films and other nano-structured polymeric materials.

This research has been performed in collaboration with T.S. Gates (NASA Langley).

Corona Poling of Partially Cured Polyimide

Cheol Park

In-situ poling and imidization of the partially cured (β-CN)APB/ODPA was studied in an attempt to maximize the degree of dipolar orientation and the resultant piezoelectric response. The dielectric relaxation strength, remnant polarization, and piezoelectric responses were evaluated as a function of the poling profile. The partially cured, corona-poled polymers exhibited higher dielectric relaxation strength ($\delta\varepsilon$), remnant polarization (P_r), and piezoelectric strain coefficient (d_33) than the fully cured, conventionally poled ones.

Application of the in-situ poling and imidization of partially cured polyimides for amorphous polyimides containing higher dipolar concentration will be investigated.

This research was performed in collaboration with Zoubeida Ounaies (Virginia Commonwealth University), Kristopher E. Wise (ICASE), and Joycelyn S. Harrison (NASA Langley).

Single Wall Carbon Nanotube Polymer Composites

Cheol Park

Carbon nanotubes are of great interest because of their unique electronic and mechanical properties combined with their chemical stability. Single wall carbon nanotubes (SWNTs), however, have been rarely used as an electrical or mechanical inclusion in a polymer matrix mainly because of the difficulty of efficient dispersion. A novel process to effectively disperse SWNTs in an aromatic polymer was developed. This process involves an in-situ polymerization of monomers of interest in the presence of sonication during the polymerization process. The goal of this study is to develop a method to disperse SWNTs into polymer matrices on a nanoscale level. The resultant SWNT-polymer nanocomposite exhibited significant conductivity enhancement (10^{10} order of magnitude) at a very low loading (0.1 wt%) without sacrificing significant optical transmission. Mechanical properties as well as thermal stability mechanical properties were also improved with the increase of the SWNT incorporation. The SWNT-polymer nanocomposites are useful in aerospace and terrestrial applications.

SWNT/polymer nanocomposites will be further characterized microscopically (SPM, HRTEM, and HRSEM). A combined experimental and theoretical study will be performed to understand the nature of the interaction and identifying new complexes with improved properties.

This research was performed in collaboration with Zoubeida Ounaies (Virginia Commonwealth University), Sarah J. Frankland (ICASE), Kristopher E. Wise (ICASE), Greg Odegard (ICASE), Tom Gates (NASA Langley), Sharon E. Lowther (NASA Langley), Peter Lillehei (NASA Langley), Mia Siochi (NASA Langley), Joycelyn S. Harrison (NASA Langley), Alice Chang (Lockheed-Martin), Roy Crooks (Lockheed-Martin), Neal D. Evans and Edward A. Kenik (Oak Ridge National Laboratory), Jim Bentley (ORNL), and Satish Kumar (Georgia Tech).

Scanning Electron Microscopy of Carbon Nanotube Materials

Jason Rouse

A central difficulty in analyzing the quality of polymer/carbon nanotube composites is the ability to accurately determine the size of the nanotube materials in the composite, the uniformity of their dispersion,

and their relative orientation. While relative average orientation can be probed by polarized Raman spectroscopy and optical microscopy can be used to identify very poorly dispersed nanotube samples, the ability to characterize highly dispersed nanotube samples has mostly relied on transmission electron microscopy (TEM). A major drawback of TEM is the time consuming process of preparing highly uniform ultrathin ($\tilde{1}5$ nm) samples for imaging. With the advent of new high-resolution scanning electron microscopes, the ability to image nanotubes in the polymer matrix without time consuming sample preparation is being investigated.

Currently, polymer/carbon nanotube composites with varying nanotube loading levels, different polymer matrixes, and produced under multiple processing conditions are being imaged. Early results indicate that small changes in imaging parameters can dramatically affect the quality of the images obtained.

This research is perfórmed in collaboration with P.T. Lillehei and Denis Working (NASA Langley), and Cheol Park (ICASE).

Stepwise Assembly of Polymer/Carbon Nanotube Multilayered Films

Jason Rouse

An area of difficulty in forming polymer/carbon nanotube composites is the ability to sufficiently disperse the carbon nanotubes in the polymer matrix. Additionally, at high nanotube loading the high viscosity of the resulting polymer/carbon nanotube melt makes processing difficult. In order to overcome these difficulties, we have focused on the stepwise assembly of polymer/carbon nanotube films using molecular interactions. By forming films at the nanometer level, it is possible to investigate film structures that can not be constructed using bulk processing techniques.

As a starting point for the formation of polymer/single-walled carbon nanotube films, we explored the use of electrostatic interactions. The formation of thin, uniform films by the sequential adsorption of polyionic species of opposite charge is an area of significant research interest. We have found that the oxidative procedure used to remove amorphous carbon during the purification of carbon nanotubes also results in the formation of oxidized defects on the tubes themselves. These oxidized groups allow carbon nanotube bundles to act as polyionic species. Atomic force and scanning electron microscopies revealed that the sequential absorption of the cationic poly(diallyldimethylammonium chloride) followed by single walled carbon nanotubes results in the formation of dense films of overlapping nanotubes.

Future work will involve the characterization of the mechanical and electrical properties of these films. Additionally, replacement of poly(diallyldimethylammonium chloride) with a more thermally and mechanically stable polymer will be explored.

This work was done in collaboration with P.T. Lillehei (NASA Langley).

Formation of Novel Organic-inorganic Electroactive Composites

Jason Rouse

The rigors of low earth orbit require materials that possess a unique combination of physical properties. Resistance to atomic oxygen and ultraviolet radiation and the ability to tolerate large temperature changes are required. A material that possesses these attributes is the inorganic-organic polymer poly(dimethlysiloxane) (PDMS). Unfortunately, PDMS lacks functional groups that respond to electrical fields. The incorporation of such groups into PDMS is the focus of this research.

Novel PDMS-based hybrid composites were prepared by the tin-catalyzed condensation of cyanoethyltriethoxysilane with hydroxy-terminated PDMS oligomers. Films prepared at low catalyst concentration resulted in the phase-separation of the silicate into micron-sized spherical particles. These films were flexible, thermal robust, and responded to electrical fields. Measurements revealed that the dielectric constant

appeared to be frequency independent in the range 100Hz–100kHz, possibly the result of the phase separation. Electrostatic forces dominated the strain mechanism, where the overall strain response was proportional to E2, and was dictated by the dielectric constant of the composite and the driving voltage.

We are currently preparing composites with a higher loading of catalyst to retard phase separation.

This research is conducted in collaboration with Zoubeida Ounaies (Virginia Commonwealth University), Mia Siochi (NASA Langley), and Peter Lillehei (NASA Langley).

Low-color Polyimides for Space Applications
Kent A. Watson

NASA has several space applications that currently use or are evaluating polyimides. These include thin films as membranes on antennas, concentrators, coatings on second-surface mirrors, solar sails, sunshades, thermal/optical coatings and multi-layer thermal insulation blanket materials. Depending on the application, the film will require a unique combination of properties. These may include atomic oxygen resistance, ultraviolet and vacuum ultraviolet radiation resistance, low color/low solar absorption and high mechanical properties (strength, modulus, and toughness). 2,3,3',4'-biphenyltetracarboxylic dianhydride (a-BPDA) was investigated as a dianhydride for the synthesis and characterization of a series of polyimides. Polyimides derived from a-BPDA were thought to offer an attractive combination of properties such as low color, good solubility, high thermal emissivity, low solar absorptivity, and high tensile properties. This work was performed to obtain fundamental information on chemical structure/property relationships that could lead to the development of improved films for space use.

We successfully prepared a series of polyimides derived from a-BDPA and compared the materials with the corresponding 3,3'4,4'-biphenyltetracarboxylic dianhydride (s-BPDA). a-BPDA was less reactive with aromatic diamines than the s-BPDA. Polyimides from a-BPDA had higher glass transition temperatures, less color (higher optical transparency), and lower thin film tensile properties than polyimides derived from s-BPDA. A polyimide derived from a-BPDA and 1,3-bis(3-aminophenoxy)benzene (APB) had the lowest color of all polyimides prepared. Advantage of this material when compared to state-of-the-art polyimides currently in use is the potentially much lower cost of the material.

Future work includes continued evaluation of the polyimide prepared from a-PBDA and APB for potential use as a low-color material for space applications. Future work also includes the incorporation of single-wall carbon nanotubes into the most promising materials in order to provide sufficient conductivity to mitigate static charge build-up.

This work was performed in collaboration with Paul Hergenrother, Joseph Smith, Jr., and John Connell (NASA Langley) and R. Yokota (Institute of Space and Astronautical Science).

Organic Nanocomposites from Functionalized Carbon Nanotubes
Kent A. Watson

Thin film polymer materials represent enabling technology for future spacecraft. These spacecraft include large ultra-lightweight space structures, space-based observatories, and solar sails. Currently no materials exist which possess the desired combination of properties necessary to perform in these missions. Spacecraft in low Earth orbit (LEO) typically have lifetimes of five to ten years and during this time the materials are bombarded with ultraviolet (UV) and vacuum ultraviolet (VUV) radiation, atomic oxygen (AO), micrometeroids, proton radiation, and electron radiation. Materials have recently emerged that show improved resistance to AO, UV, and VUV radiation. However, all of these new materials are insulators (i.e., nonconducting). Due to charged species being present in the space environment, these polymers can build up

significant electrical charges that can eventually lead to sparking or electrical arcing. Transfer of the electrical charge from the film-based material to the main body of the spacecraft can cause catastrophic damage to computers and sensitive electronic devices. Recent work has involved incorporation of single-wall carbon nanotubes (SCNT) into polymeric materials to add sufficient conductivity to mitigate static charge build-up. One main obstacle to using SCNTs is their difficulty in dispersing in an organic medium. They are both insoluble in organic solvents and the SCNTs tend to agglomerate into bundles. To overcome these difficulties we will investigate the preparation of organic nanocomposites using functionalized SCNTs.

We are currently investigating different methods of functionalizing SCNTs primarily by taking advantage of functional groups already existing on the surface of the nanotubes. Organic functional groups are formed on the surface of the nanotubes during purification (acid treatment). Oligomer or polymer chains can be chemically bound to the surface of the nanotubes at these functional group sites. Attachment of oligomer or polymeric organic moieties should aid in dispersion of the SCNTs in organic solvents and also show improved compatibility with host polymers. Our preliminary work has involved the preparation of functionalized SCNTs and incorporation into space durable polymers. We have prepared functionalized SCNTs that contain small molecules as well as oligomeric groups attached to the nanotubes surface.

Current and future work includes exploring additional methods for SCNT functionalization and characterization of the functionalized SCNTs. Characterization of the polymer/functionalized SCNT nanocomposites will also be investigated.

This work is being performed with the collaboration of John Connell (NASA Langley) and Y. Sun (Clemson University).

Modeling Nanotube Dispersion in a Polymer Matrix
Kristopher Wise

A key enabling technology for the application of carbon nanotubes in practical devices is the ability to disperse them in a polymer matrix. Currently, kinetically stable (short lived) nanotube-polymer solutions can be prepared by a variety of traditional stirring/mixing methods. Unfortunately these solutions eventually phase separately due to the strength of the tube-tube (relative to the polymer-tube) interactions. Achieving thermodynamically stable nanotube-polymer composite systems will require enhancing the attractive interaction between the matrix and nanotubes.

Using a combination of high-level *ab initio* (Hartree-Fock and Density Functional Theory) and classical (Molecular Dynamics and Monte Carlo) simulation methods, we are studying the effect of varying the chemical composition of the polymer on its ability to stabilize nanotube dispersions. Based on preliminary results, we have proposed a mechanism involving the formation of an electron donor/acceptor complex between particular functional groups on the polymer and the nanotube.

Ongoing work is proceeding in two primary directions: expanding the types of polymer systems being studied and developing new simulation methodologies. Based on what has been learned to this point, we have a number of new polymer systems which we will be testing both experimentally and through simulation. We are also working on ways of expanding our simulation capabilities to encompass larger composite systems and longer simulation times.

This work is being performed in collaboration with Cheol Park (ICASE), Zoubeida Ounaies (Virginia Commonwealth University), and Mia Siochi and Joycelyn S. Harrison (NASA Langley).

Development of Facilities for Characterizations of Electromechanical Properties of Electroactive Polymer-based Materials and Devices

Tian-Bing Xu

Electroactive polymers (EAP), which change shape as an electric field is applied, can be used in many areas such as artificial muscles and organs, smart materials for vibration and noise control, electromechanical actuators and sensors for robots, acoustic transducers used for underwater navigation and medical imaging, and fluid pumps and valves. Compared with piezoceramic and magnetostrictive actuator materials, polymers have many advantages such as flexibility, easy processing, light weight, and low cost. Polymeric materials can also withstand a large dimensional change (strain) without fatigue and are quite robust. Recently, a Graft elastomer-based EAP with giant strain, relatively high elastic modulus, and high energy density has been developed at NASA Langley. There are, however, no commercialized methods for electromechanical property characterizations in the EAP films. In order to keep world leadership in the field of research on EAP and EAP-based devices, it is necessary to develop/install the unique world leader facilities at NASA Langley to match the needs of characterization of electromechanical response on the EAP films and EAP based electromechanical devices.

A transverse strain measurement set-up (Strain response in lateral direction of the films), a longitudinal strain set-up (Strain response in the thickness direction), and a force measurement set-up for electromechanical response in EAP films have been designed and fabricated in this duration. The performances of these facilities are under evaluation. On the other hand, a four probes conductivity measurement station has been installed and evaluated. It works fine. In addition, the laser vibrometer based displacement/actuation measurement set for micromachined actuators has been designed and the laser vibrometer is selected (under order process). There unique facilities can greatly increase our capability to do/lead research on EAP materials and EAP-based devices.

We are going to characterize the electromechanical response of EAP films at different process conditions and compositions to optimize/improve the electromechanical properties of the EAP films after calibrating the new facilities. On the other hand, we also plan to develop the EAP-based actuators and micro-electromechanical systems (MEMS) for aerospace applications.

This work is accomplished in collaboration with Ji Su and Joycelyn S. Harrison (NASA Langley).

REPORTS AND ABSTRACTS

Stals, Linda: *The solution of radiation transport equations with adaptive finite elements.* ICASE Report No. 2001-29, (NASA/CR-2001-211230), October 15, 2001, 20 pages. Proceedings of the Tenth Copper Mountain Conference on Multigrid Methods.

We compare the performance of an inexact Newton-multigrid method and Full Approximation Storage multigrid when solving radiation transport equations. We also present an adaptive refinement algorithm and explore its impact on the solution of such equations.

Shin, Jong-Yeob: *Analysis of linear parameter varying system models based on reachable sets.* ICASE Report No. 2001-30, (NASA/CR-2001-211231), October 24, 2001, 22 pages. To be submitted to American Control Conference (ACC) 2002.

This paper presents the analysis method of quasi-LPV models, comparing the ellipsoid set which contains the reachable set of a nonlinear system to define which quasi-LPV model is less conservative to represent the nonlinear dynamics. Three quasi-LPV models are constructed from a nonlinear model using three different methods, to facilitate synthesis of an LPV controller for the nonlinear system. The comparison results of closed-loop system performance with synthesized LPV controllers correspond to the analysis results of quasi-LPV models.

Povitsky, Alex: *Three-dimensional flow in cavity at yaw.* ICASE Report No. 2001-31, (NASA/CR-2001-211232), October 24, 2001, 23 pages. AIAA Paper No. 01-2847.

This study is motivated by three-dimensional flows about protrusions and cavities with an arbitrary angle between the external flow and rigid elements. The novel type of a "building block" cavity flow is proposed where the cavity lid moves along its diagonal (Case A). The proposed case is taken as a typical representative of essentially three-dimensional highly separated vortical flows having simple single-block rectangular geometry of computational domain. Computational results are compared to the previous studies where the lid moves parallel to the cavity side walls (Case B). These 3-D lid-driven cavity flows are studied by numerical modeling using second-order upwind schemes for convective terms. The volume and plane integrals of primary and transversal momentum are introduced to compare cases in a quantitative way. For the laminar flow in the cubic cavity, the integral momentum of the secondary flow (which is perpendicular to the lid direction) is about an order of magnitude larger than that in Case B. In Case A, the number of secondary vortices substantially depends on the Re number. The secondary vortices in the central part of the cavity in Case A distinguishes it from Case B, where only corner secondary vortices appear. For a rectangular 3-D 3:1:1 cavity the integral momentum of the secondary flow in Case A is an order of magnitude larger than that in the benchmark cases. The flowfield in Case A includes a curvilinear separation line and non-symmetrical vortices which are discussed in the paper. The estimated Gortler number is approximately 4.5 times larger in Case A than that in Case B for the same Re number. This indicates that in Case A the flow becomes unsteady for smaller Re numbers than in Case B. For developed turbulent flow in the cubic cavity, the yaw effect on amplification of secondary flow is as strong as that for the laminar flow despite the more complex vortical flow pattern in benchmark case B.

Parikh, Stavan M.: *An analysis mechanism for automation in terminal area.* ICASE Report No. 2001-32, (NASA/CR-2001-211235), October 31, 2001, 15 pages.

This paper describes an Air Traffic Simulator (ATS) that provides a simulation capability for terminal area automation. The ATS is capable of realistic terminal area modeling, automation performance and feasibility studies, and system wide fault-tolerance analysis. The ATS is evaluated through modeling of self-spacing and self-merging of aircraft following Standard Terminal Arrival (STARs). These algorithms are described in detail and preliminary analysis results are provided. The analysis exposes the limitations of the algorithms due to their integration. Possible modifications to overcome these limitations are suggested. Future work planned for the ATS is described. Overall the ATS is an easily extensible and powerful tool for preliminary analysis of new technologies.

Shin, Jong-Yeob, Gary J. Balas, and Alpay M. Kaya: *Blending methodology of linear parameter varying control synthesis of F-16 aircraft systems.* ICASE Report No. 2001-33, (NASA/CR-2001-211237), October 29, 2001, 26 pages. To be submitted to the Journal of Guidance, Control, and Dynamics.

This paper presents the design of a linear parameter varying (LPV) controller for the F-16 longitudinal axes over the entire flight envelope using a blending methodology which lets an LPV controller preserve performance level over each parameter subspace and reduces computational costs for synthesizing an LPV controller. Three blending LPV controller synthesis methodologies are applied to control F-16 longitudinal axes. Using a function substitution method, a quasi-LPV model of the F-16 longitudinal axes is constructed from the nonlinear equations of motion over the entire flight envelope, including non-trim regions, to facilitate synthesis of LPV controllers for the F-16 aircraft. The nonlinear simulations of the blending LPV controller show that the desired performance and robustness objectives are achieved across all altitude variations.

Prieto, Manuel, Ruben S. Montero, and Ignacio M. Llorente: *A parallel multigrid solver for viscous flows on anisotropic structured grids.* ICASE Report No. 2001-34, (NASA/CR-2001-211238), October 31, 2001, 24 pages. To be submitted to Parallel Computing.

This paper presents an efficient parallel multigrid solver for speeding up the computation of a 3-D model that treats the flow of a viscous fluid over a flat plate. The main interest of this simulation lies in exhibiting some basic difficulties that prevent optimal multigrid efficiencies from being achieved. As the computing platform, we have used Coral, a Beowulf-class system based on Intel Pentium processors and equipped with GigaNet cLAN and switched Fast Ethernet networks. Our study not only examines the scalability of the solver but also includes a performance evaluation of Coral where the investigated solver has been used to compare several of its design choices, namely, the interconnection network (GigaNet versus switched Fast-Ethernet) and the node configuration (dual nodes versus single nodes). As a reference, the performance results have been compared with those obtained with the NAS-MG benchmark.

Huyse, Luc, and Robert W. Walters: *Random field solutions including boundary condition uncertainty for the steady-state generalized Burgers equation.* ICASE Report No. 2001-35, (NASA/CR-2001-211239), October 29, 2001, 30 pages. To be submitted to the Journal of Fluid Mechanics.

CFD results are subject to considerable uncertainty associated with the operating conditions. Even when the operational uncertainty is omitted under very controlled circumstances during wind tunnel experiments, substantial disagreement between experimental and CFD results persists. This discrepancy must be

attributed to model uncertainty. This report discusses the various sources of uncertainty. The need for advanced uncertainty modeling is illustrated by means of a computationally inexpensive 1-D Burgers equation model. We specifically address the uncertainty due to missing variables (inexact or incomplete differential equations). To this extent a random field model is used for the viscosity and the fundamental differences between the solutions of the stochastic differential equations and a simple random variable model is highlighted. The Burgers equation theoretically needs to be integrated over an infinite domain. In a deterministic approach, the integration domain is cut off at some far field boundary. This truncation effectively ignores all variability outside this far field boundary. We present a practical treatment for the uncertainty on the boundary conditions. The results indicate that ignoring the boundary condition uncertainty dramatically underestimates the variance of the velocity in the interior of the domain.

Little, Mark E., and Martin E. Kordesch: *Band-gap engineering in sputter deposited amorphous/microcrystalline $Sc_xGa_{1-x}N$.* ICASE Report No. 2001-36, (NASA/CR-2001-211241), November 29, 2001, 11 pages. To be submitted to the Proceedings of the MRS Fall Meeting.

Reactive sputtering was used to grow thin films of $Sc_xGa_{1-x}N$ with scandium concentrations of 20%-70% on quartz substrates at temperatures of 300-675 K. X-ray diffraction (XRD) of the films showed either weak or no structure, suggesting the films are amorphous or microcrystalline. Optical absorption spectra were taken of each sample and the optical band gap was determined. The band gap varied linearly with increasing Ga concentration between 2.0 and 3.5 eV. Ellipsometry was used to confirm the band gap measurements and provide optical constants in the range 250-1200 nm. ScN and GaN have different crystal structures (rocksalt and wurzite, respectively), and thus may form a heterogeneous mixture as opposed to an alloy. Since the XRD data were inconclusive, bilayers of ScN/GaN were grown and optical absorption spectra taken. A fundamental difference in the spectra between the bilayer films and alloy films was seen, suggesting the films are alloys, not heterogeneous mixtures.

Hart, Roger C., G.C. Herring, and R. Jeffrey Balla: *Common-path heterodyne laser-induced thermal acoustics for seedless laser velocimetry.* ICASE Report No. 2001-37, (NASA/CR-2001-211252), March 7, 2002, 12 pages. To be submitted to Optic Letters.

We demonstrate the use of a novel technique for the detection of heterodyne laser-induced thermal acoustics signals, which allows the construction of a highly stable seedless laser velocimeter. A common-path configuration is combined with quadrature detection to provide flow direction, greatly improve robustness to misalignment and vibration, and give reliable velocity measurement at low flow velocities. Comparison with Pitot tube measurements in the freestream of a windtunnel shows root-mean-square errors of 0.67 m/s over the velocity range 0-55 m/s.

Zhang, Yong-Tao, and Chi-Wang Shu: *High order WENO schemes for Hamilton-Jacobi equations on triangular meshes.* ICASE Report No. 2001-38, (NASA/CR-2001-211256), December 26, 2001, 36 pages. Submitted to the SIAM Journal on Scientific Computing.

In this paper we construct high order weighted essentially non-oscillatory (WENO) schemes for solving the nonlinear Hamilton-Jacobi equations on two-dimensional unstructured meshes. The main ideas are nodal based approximations, the usage of monotone Hamiltonians as building blocks on unstructured meshes, nonlinear weights using smooth indicators of second and higher derivatives, and a strategy to choose diversified smaller stencils to make up the bigger stencil in the WENO procedure. Both third-order and fourth-order

WENO schemes using combinations of second-order approximations with nonlinear weights are constructed. Extensive numerical experiments are performed to demonstrate the stability and accuracy of the methods. High-order accuracy in smooth regions, good resolution of derivative singularities, and convergence to viscosity solutions are observed.

Xu, Kun: *Regularization of the Chapman-Enskog expansion and its description of shock structure.* ICASE Report No. 2001-39, (NASA/CR-2001-211268), December 26, 2001, 11 pages. To be submitted to Physics of Fluids.

In the continuum transition flow regime, we propose to truncate the Chapman-Enskog expansion of the Boltzmann equation to the Navier-Stokes order only without going to the Burnett or super Burnett orders. However, the local particle collision time has to be generalized to depend not only on the local macroscopic flow variables, but also their gradients in the rarefied gas regime. Based on the gas-kinetic BGK model, the relation between the conventional collision time and the general one is obtained. More specificially, a generalized constitutive relation for stress and heat flux is proposed. This new model is applied to the study of argon gas shock structure. There is good agreement between the predicted shock structure and experimental results for a wide range of Mach numbers.

Hu, Fang Q., and Harold L. Atkins: *Eigensolution analysis of the discontinuous Galerkin method with non-uniform grids, part I: One space dimension.* ICASE Report No. 2001-40, (NASA/CR-2001-211269), December 26, 2001, 35 pages. To be submitted to the Journal of Computational Physics.

We present a detailed study of spatially propagating waves in a discontinuous Galerkin scheme applied to a system of linear hyperbolic equations. We start with an eigensolution analysis of the semi-discrete system in one space dimension with uniform grids. It is found that, for any given order of the basis functions, there are at most two spatially propagating numerical wave modes for each physical wave of the Partial Differential Equations (PDE). One of the modes can accurately represent the physical wave of the PDE and the other is spurious. The directions of propagation of these two numerical modes are opposite, and, in most practical cases, the spurious mode has a large damping rate. Furthermore, when an exact characteristics split flux formula is used, the spurious mode becomes non-existent. For the physically accurate mode, it is shown analytically that the numerical dispersion relation is accurate to order $2p+2$ where p is the highest order of the basis polynomials. The results of eigensolution analysis are then utilized to study the effects of a grid discontinuity, caused by an abrupt change in grid size, on the numerical solutions at either side of the interface. It is shown that, due to "mode decoupling," numerical reflections at grid discontinuity, when they occur, are always in the form of the spurious non-physical mode. Closed form numerical reflection and transmission coefficients are given and analyzed. Numerical examples that illustrate the analytical findings of the paper are also presented.

Jow, Kenny G., and Theo J. Dingemans: *Liquid crystals derived from 2-phenyl-isoindoles.* ICASE Report No. 2001-41, (NASA/CR-2001-211270), January 15, 2002, 18 pages. To appear in Liquid Crystals.

2-Phenyl-isoindole was investigated as the rigid core unit in a series of asymmetric mesogenic molecules. When the 2-phenyl-isoindole core was terminated with a hexyl tail, no mesophase formation could be observed. When 4-n-(tridecafluorohexyl) was used, however, we observed both monotropic and enantiotropic phase behavior. We found that most functionalities at the anhydride 5-position results in the formation of smectic A (SmA) phases in the temperature range of 70-180°C. Functionalities at the anhydride 4-position

suppress mesophase formation. Large substituents (-Br, -NO_2) and symmetric substitution patterns (5,6-dichloro, 4,7-dichloro and 4,5,6,7-tetrachloro) on the anhydride moiety increase the melting point and destabilize the mesophase. Temperature dependent X-ray diffraction experiments suggest an interdigitated SmA packing for this family of compounds.

Heggernes, P., S.C. Eisenstat, G. Kumfert, and A. Pothen: *The computational complexity of the Minimum Degree algorithm.* ICASE Report No. 2001-42, (NASA/CR-2001-211421), January 15, 2002, 16 pages. Proceedings of the Norwegian Computer Science Conference NIK 2001.

The Minimum Degree algorithm, one of the classical algorithms of sparse matrix computations, is widely used to order graphs to reduce the work and storage needed to solve sparse systems of linear equations. There has been extensive research involving practical implementations of this algorithm over the past two decades. However, little has been done to establish theoretical bounds on the computational complexity of these implementations. We study the Minimum Degree algorithm, and prove time complexity bounds for its widely used variants.

Harrison, J.S., and Z. Ounaies: *Piezoelectric polymers.* ICASE Report No. 2001-43, (NASA/CR-2001-211422), March 28, 2002, 31 pages. To appear in the Encyclopedia of Smart Materials, John Wiley, December 2001.

The purpose of this review is to detail the current theoretical understanding of the origin of piezoelectric and ferroelectric phenomena in polymers; to present the state-of-the-art in piezoelectric polymers and emerging material systems that exhibit promising properties; and to discuss key characterization methods, fundamental modeling approaches, and applications of piezoelectric polymers. Piezoelectric polymers have been known to exist for more than forty years, but in recent years they have gained notoriety as a valuable class of smart materials.

Carpenter, Mark H., David Gottlieb, and Chi-Wang Shu: *On the conservation and convergence to weak solutions of global schemes.* ICASE Report No. 2001-44, (NASA/CR-2001-211423), March 1, 2002, 20 pages. To appear in the Journal of Scientific Computing.

In this paper we discuss the issue of conservation and convergence to weak solutions of several global schemes, including the commonly used compact schemes and spectral collocation schemes, for solving hyperbolic conservation laws. It is shown that such schemes, if convergent boundedly almost everywhere, will converge to weak solutions. The results are extensions of the classical Lax-Wendroff theorem concerning conservative schemes.

Wu, Xuesong, and Meelan Choudhari: *Linear and nonlinear instabilities of Blasius boundary layer perturbed by streamwise vortices part II: Intermittent instability induced by long-wavelength Klebanoff modes.* ICASE Report No. 2001-45, (NASA/CR-2001-211424), March 8, 2002, 46 pages. To be submitted to the Journal of Fluid Mechanics.

We present theoretical results on the stability properties of a Blasius boundary layer perturbed by Klebanoff distortions with a relatively long spanwise scale. Even relatively weak Klebanoff modes can alter the near-wall curvature of the underlying flow by O(1) and, hence, introduce linear instabilities with larger characteristic growth rates and frequencies than those of the Tollmien-Schlichting waves in an unpertubed Blasius flow. A localised distortion supports both sinuous and varicose modes of instability, with the growth

rates of the sinuous modes being likely to be larger, in general. Overall, the instability is intermittent in time and localised in space, being confined to a finite part of the Klebanoff mode cycle and to a specific window(s) along the streamwise direction. A spanwise periodic distortion supports spatially quasi-periodic modes (via the parametric resonance mechanism), which may be viewed as modified T-S waves with excess growth rates when the Klebanoff modes are weak. In spite of the simplifications involved in this theory, its predictions appear qualitatively consistent with some of the unusual characteristics of the high-frequency wavepackets observed during previous experiments. The nonlinear development of a localised sinuous mode is followed across a sequence of asymptotic regimes using the non-equlibrium critical-layer theory.

Walters, Robert W., and Luc Huyse: *Uncertainty analysis for fluid mechanics with applications.* ICASE Report No. 2002-1, (NASA/CR-2002-211449), March 29, 2002, 50 pages.

This paper reviews uncertainty analysis methods and their application to fundamental problems in fluid dynamics. Probabilitic (Monte-Carlo, Moment methods, Polynomial Chaos) and non-probabilistic methods (Interval Analysis, Propagation of error using sensitivity derivatives) are described and implemented. Results are presented for a model convection equation with a source term, a model non-linear convection-diffusion equation; supersonic flow over wedges, expansion corners, and an airfoil; and two-dimensional laminar boundary layer flow.

Rubinstein, R., and Guowei He: *The Eulerian time correlation function in homogeneous isotropic turbulence.* ICASE Report No. 2002-2, (NASA/CR-2002-211450), March 29, 2002, 14 pages. To appear in the Proceedings of the International Workshop on Statistical Theories and Computational Approaches to Turbulence.

Two general models are proposed for the Eulerian time correlation function in homogeneous isotropic turbulence. The first is based on continued fraction approximations to its Laplace transform, and the second is based on random sweeping by a possibly non-Gaussian velocity field. Both models can give reasonable quantitative agreement with DNS data for moderate time separations over which the time correlation functions at different wavenumbers exhibit a common self-similar form.

Geser, Alfons: *Loops of superexponential lengths in one-rule string rewriting.* ICASE Report No. 2002-3, (NASA/CR-2002-211451), March 27, 2002, 16 pages. To be submitted to the International Conference on Rewriting Techniques and Applications.

Loops are the most frequent cause of non-termination in string rewriting. In the general case, non-terminating, non-looping string rewriting systems exist, and the uniform termination problem is undecidable. For rewriting with only one string rewriting rule, it is unknown whether non-terminating, non-looping systems exist and whether uniform termination is decidable. If in the one-rule case, non-termination is equivalent to the existence of loops, as McNaughton conjectures, then a decision procedure for the existence of loops also solves the uniform termination problem. As the existence of loops of bounded lengths is decidable, the question is raised how long shortest loops may be. We show that string rewriting rules exist whose shortest loops have superexponential lengths in the size of the rule.

Krueger, Ronald, and Pierre J. Minguet: *Influence of 2D finite element modeling assumptions on debonding prediction for composite skin-stiffener specimens subjected to tension and bending.* ICASE Report No. 2002-4, (NASA/CR-2002-211452), March 29, 2002, 35 pages. To be presented at the International Conference on Composite Structures.

The influence of two-dimensional finite element modeling assumptions on the debonding prediction for skin-stiffener specimens was investigated. Geometrically nonlinear finite element analyses using two-dimensional plane-stress and plane-strain elements as well as three different generalized plane strain type approaches were performed. The computed deflections, skin and flange strains, transverse tensile stresses and energy release rates were compared to results obtained from three-dimensional simulations. The study showed that for strains and energy release rate computations the generalized plane strain assumptions yielded results closest to the full three-dimensional analysis. For computed transverse tensile stresses the plane stress assumption gave the best agreement. Based on this study it is recommended that results from plane stress and plane strain models be used as upper and lower bounds. The results from generalized plane strain models fall between the results obtained from plane stress and plane strain models. Two-dimensional models may also be used to qualitatively evaluate the stress distribution in a ply and the variation of energy release rates and mixed mode ratios with delamination length. For more accurate predictions, however, a three-dimensional analysis is required.

INTERIM REPORTS

Eidson, Thomas M., and Merrell L. Patrick: *ICASE Workshop on Programming Computational Grids.* ICASE Interim Report No. 38, (NASA/CR-2001-211224), October 15, 2001, 21 pages.

A workshop on Programming Computational Grids for distributed applications was held on April 12-13, 2001 at ICASE, NASA Langley Research Center. The stated objective of the workshop was to define, discuss, and clarify issues critical to the advancement of Problem Solving Environments/Computational Frameworks for solving large multi-scale, multi-component scientific applications using distributed, heterogeneous computing systems. This report documents a set of recommendations for NASA that suggest an approach for developing an application development environment that will meet future application needs.

Munoz, Cesar, and Micaela Mayero: *Real automation in the field.* ICASE Interim Report No. 39, (NASA/CR-2001-211271), January 22, 2002, 14 pages.

We provide a package of strategies for automation of non-linear arithmetic in PVS. In particular, we describe a simplification procedure for the field of real numbers and a strategy for cancellation of common terms.

ICASE COLLOQUIA

Name/Affiliation/Title	Date
Achi Brandt, The Weizmann Institute of Science, Israel "Multiscale Computational Methods for Molecular Dynamics"	October 2
Ken Schwaber, Advanced Development Methods, Inc. ICASE Series on Modern Programming Practices: "Agile Processes: A Case Study of a Scrum Project"	October 2
Gregory Carman, University of California, Los Angeles ICASE Series on Morphing: "Investigating the Passive Damping Properties of Active Materials"	October 3
Michael Hill, Object Mentor, Inc. ICASE Series on Modern Programming Practices: "The Four Keys to Test-first Design: Laziness, Resentment, Xenophobia, and Guile"	October 4
George Haller, Brown University "Lagrangian Coherent Structures and their Control"	October 22
Thomas Bewley, University of California, San Diego ICASE Series on Morphing: "Adjoint and Riccati: Essential Tools in the Analysis and Control of Transitional and Turbulent Flow Systems"	October 23
Terrence Weisshaar, Purdue University ICASE Series on Morphing: "Aeroelastic Tailoring for Energy Efficient Morphing Aircraft – Finding the Right Stuff"	October 25
Dieter Wolf, Argonne National Laboratory ICASE Series on Nanotechnology: "Plastic Deformation of Nanocrystalline Materials by Molecular-dynamics Simulation"	October 30
Inderjit Chopra, University of Maryland, College Park ICASE Series on Morphing: "Review on the Status of Application of Smart Structures Technology to Rotorcraft Systems"	October 31
Michael Two, ThoughtWorks, Inc. ICASE Series on Modern Programming Practices: "Continuous Integration"	November 5

Name/Affiliation/Title	Date
Joel Grasmeyer, AeroVironment, Inc. ICASE Series on Morphing: "Perspectives on Micro Air Vehicles and Electronic Packaging"	November 9
Tony Ingraffea, Cornell University ICASE Series on Nanotechnology: "A Multiscale Modeling Approach to Crack Initiation in Aluminum Polycrystals"	November 13
David Geohegan, Oak Ridge National Laboratory "Time-resolved Growth Studies and Applications of Single-wall Carbon Nanotubes"	November 14
Richard James, University of Minnesota ICASE Series on Nanotechnology: "Deforming Films of Active Materials: New Concepts for Producing Motion at Small Scales using Applied Fields"	November 15
Reeti Katoch-Rouse, Lehigh University "Controlled Reductive Cyclization for the Synthesis of dihydrobenzofurans/ Stereocontrolled Preparation of Functionalized Dienes for Decalin Synthesis"	November 16
Deborah Mayo, Virginia Polytechnic Institute and State University ICASE Series on Risk-based Design: "Learning from Error and an Error Statistical Philosophy of Science"	November 16
Anatole Beck, University of Wisconsin, Madison "Some Interesting Anomalies in the Uniqueness of Solutions of Differential Equations"	November 20
Armen Der Kiureghian, University of California, Berkeley ICASE Series on Risk-based Design: "Algorithms for Reliability-based Optimal Structural Design"	November 26
David McDowell, Georgia Institute of Technology ICASE Series on Nanotechnology: "Computational Modeling of Plasticity and Fracture at Microstructure Scales"	November 29
Mohammad Khalessi, Unipass Technologies ICASE Series on Risk-based Design: "Probabilistic Technology at PredictionProbe, Inc."	December 3

Name/Affiliation/Title	Date
Satish Kumar, Georgia Institute of Technology "Films, Fibers, and Coatings from Carbon Nano Tubes, Nano Fibers, and their Composites with Polymers"	December 5
Kyung Choi, The University of Iowa ICASE Series on Risk-based Design: "Advances in Reliability-based Design Optimization and Probability Analysis – Part I"	December 10
Kyung Choi, The University of Iowa ICASE Series on Risk-based Design: "Advances in Reliability-based Design Optimization and Probability Analysis – Part II"	December 11
Harry Dorn, Virginia Polytechnic Institute and State University ICASE Series on Multifunctional Materials: "Nanoscale Carbonaceous Building Blocks: Properties and Applications"	December 13
Do Young, Kwak KAIST, Korea "Convergence of Multigrid for Nonconforming FE and Cell-centered FD"	January 18
Kie Eom, The George Washington University "Random Field Models for Analysis of Natural and Artificial Patterns"	January 25
Emmanuel Giannelis, Cornell University "New Advances in Polymer Nanocomposites"	February 5
Boris Berkovski, Global Science and Technology, Inc. "Some New Approaches in Aeronautical Modeling"	February 6
Michael Trosset, The College of William and Mary "Uncertainty in Computational Science: First Impressions"	February 8
Brien Alkire, University of California, Los Angeles "Convex Optimization Problems Involving Autocorrelation Sequences"	February 11
Roger Ghanem, The Johns Hopkins University ICASE Series on Risk-based Design: "Propagation and Management of Uncertainty in Mechanics-based Models"	February 14
Nicholas Bailey, Cornell University ICASE Series on Nanotechnology: "Aspects of Mixed Atomistic-continuum Modeling"	February 22

Name/Affiliation/Title	Date
Dmitry Keselman, Atraxis North America, Inc. "On Some Problems of Scheduling and the Airline Network Analysis"	February 25
Luis Crespo, University of Delaware "Deterministic and Stochastic Optimal Control via Bellman's Principle"	March 4
John Gilbert, Palo Alto Research Center and MIT Laboratory for Computer Science "Smart Matter: Frontiers of Computation"	March 7
George Lauder, Harvard University ICASE Series on Morphing: "Fish Morphing: Experimental Hydrodynamics of Locomotion in Fishes"	March 15
Larry Howell, Brigham Young University "Compliant Micro Mechanism Analysis and Design"	March 25
John Renaud, University of Notre Dame ICASE Series on Risk-based Design: "Decision-based Collaborative Optimization and Estimation of Propagated Uncertainty"	March 28

OTHER ACTIVITIES

On November 6–7, 2001, ICASE/USRA and NASA Langley co-sponsored a workshop on Revolutionary Aerospace Systems Concepts for Human/Robotic Exploration of the Solar System at the Quality Inn and the Holiday Inn in Hampton, Virginia. The primary focus of this workshop was to understand how, with the incorporation of revolutionary aerospace systems concepts over the next 10–40 years, humans and machines can be synergistically combined to physically and virtually reduce the time and distance barriers associated with exploring beyond low Earth orbit. There were 85 attendees and a NASA Conference Proceedings will be published.

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